

CACHE NEWS

**News about Computers in
Chemical Engineering Education**

No. 59

Fall 2004

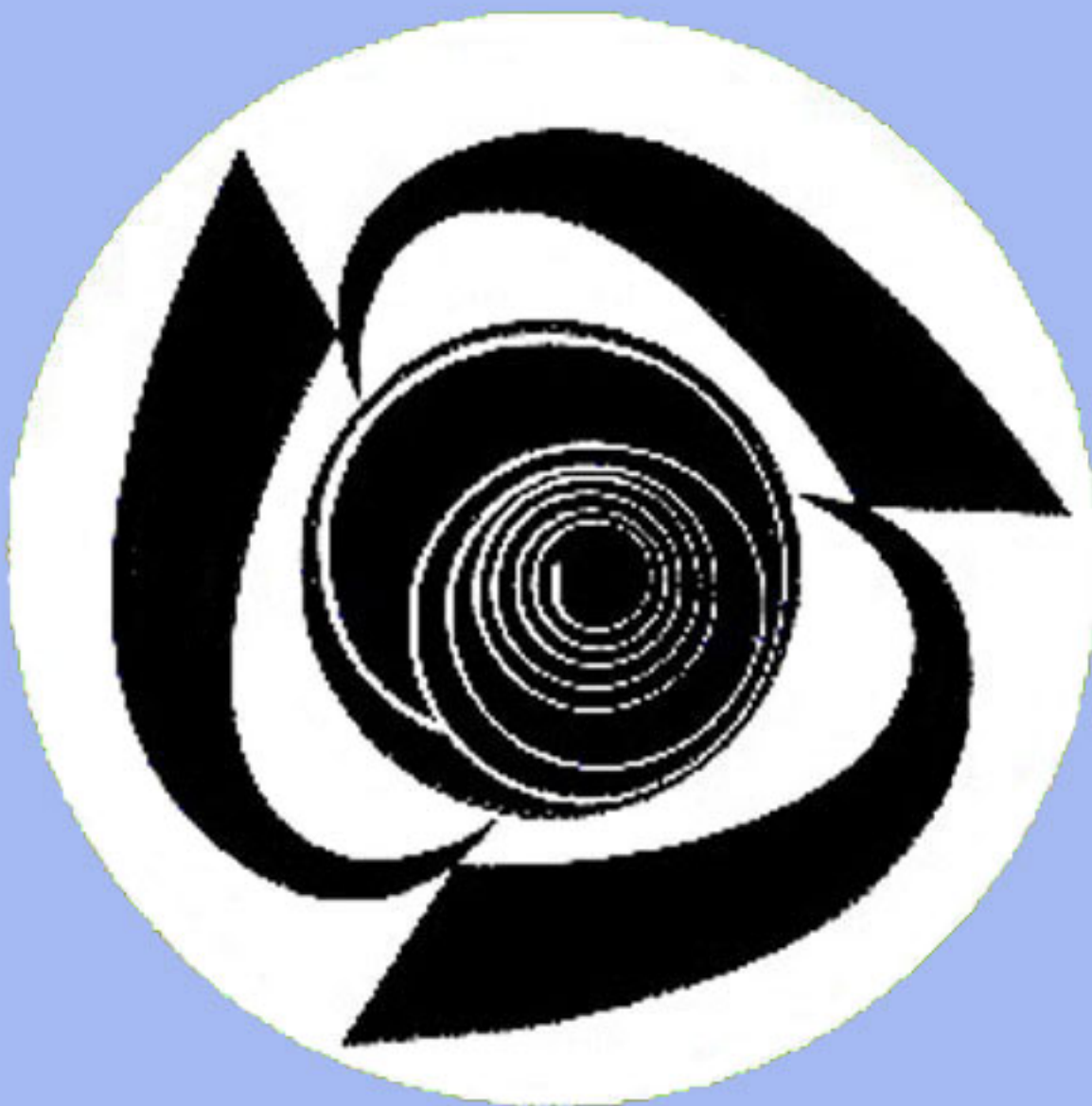


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THE CACHE CORPORATION

WHAT IS CACHE?

CACHE is a not-for-profit organization whose purpose is to promote cooperation among universities, industry and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession.

CREATION OF THE CACHE CORPORATION

During the 1960s the rapid growth of computer technology challenged educators to develop new methods of meshing the computer with the teaching of chemical engineering. In spite of many significant contributions to program development, the transferability of computer codes, even those written in FORTRAN, was minimal. Because of the disorganized state of university-developed codes for chemical engineering, fourteen chemical engineering educators met in 1969 to form the CACHE (Computer Aids for Chemical Engineering) Committee. The CACHE Committee was initially sponsored by the Commission on Education of the National Academy of Engineering and funded by the National Science Foundation. In 1975, after several successful projects had been completed, CACHE was incorporated as a not-for-profit corporation in Massachusetts to serve as the administrative umbrella for the consortium activities.

CACHE ACTIVITIES

All CACHE activities are staffed by volunteers including both educators and industrial members, and coordinated by the Board of Trustees through various Task Forces. CACHE actively solicits the participation of interested individuals in the work of its ongoing projects. Information on CACHE activities is regularly disseminated through *CACHE News*, published twice yearly.

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CACHE NEWS

The *CACHE News* is published twice a year and reports news of CACHE activities and other noteworthy developments of interest to chemical engineering educators. Persons who wish to be placed on the mailing list should notify CACHE at the aforementioned address. Contributions from CACHE representatives are welcome. This issue was edited by Christine Bailor with contributions from a number of CACHE members and representatives.

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COMMENTS FROM THE EDITORS

Tom Edgar, Peter Rony, Ed Rosen, and Scott Fogler

This issue of CACHE News (No. 59 - Fall 2004) includes a number of papers dealing with experiments in chemical engineering laboratories that relate to statistical analysis and process control. There are also several articles that deal with simulators such as employed in computational fluid dynamics (CFD). We are also pleased to include the slides from a recent WebCAST by Dr. George Stephanopoulos, which was cooperatively organized by the AIChE CAST Division and CACHE; as well as slides from Tom Edgar's plenary lecture at the ASEE Annual Meeting last June. Finally, reports on past and future conferences sponsored by CACHE are included. Of note is a new conference on systems biology (FOSBE) to be held next summer, and the report on the successfully completed FOCAPD Conference held last summer at Princeton University.

CACHE Newsletter Committee

USING THE EVOLUTIONARY OPERATION METHOD

To Optimize Gas Absorber Operation (A Statistical Method for Process Improvement)

JIMMY L. SMART

University of Kentucky • Paducah, KY 42002

Evolutionary Operation (EVOP) is a statistical tool developed for incrementally moving the operation of a dynamic process in the direction of some optimum set of conditions. The EVOP method^[1] was introduced in the late 1950s as a field application technique for improving existing industrial processes. It was to be applied to an existing manufacturing process that was currently producing acceptable product. By exploring small incremental changes in an existing set of process conditions, the process could be improved and moved in the direction of some process optimum.

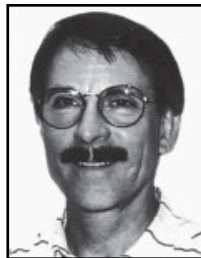
There are other advanced statistical methods, such as strategies of experimentation,^[2] simplex optimization,^[3] response surface methodology,^[4] and advanced factorial design,^[5] but they are more complex and require a great deal of training for reliable application and interpretation. Most of the methods deal with an initial strategy of experimentation when formulating a set of bench-scale experimental runs. The goal of experimental design is to minimize the number of runs while at the same time maximizing the amount of useful information.

MOTIVATION

EVOP is a simple technique that is relatively easy to apply and provides intuitive, yet statistically based results. In the chemical engineering undergraduate laboratory at the University of Kentucky, students operate a carbon dioxide scrubber to gain training in using the EVOP method. Not only do they acquire knowledge of how to design a scrubber, but they also learn how the interplay of various operating parameters affects the overall scrubbing performance of the device. Details of this student experience were previously delivered at

the annual ASEE conference in 2003.^[6]

Typically, a gas scrubber is a packed column that uses liquid media such as water to absorb and remove contaminants from polluted industrial gas streams. This scrubbing process often serves as a final process step prior to release of the "clean" air into the environment. Chemical engineering students in the undergraduate curriculum learn to design packed columns for use as air pollution control devices. Most curricula include some hands-on training with these devices in the laboratory environment. The design techniques learned by students are approximate methods based on such operating variables as column-pressure drop, packing factors, and mass transfer coefficients. These approximations often serve as a fundamental basis for design and construction of air pollution control devices, but in reality, final optimization and fine-tuning are often performed by engineers in the field on already-installed operational equipment. The EVOP technique is ideally suited for optimizing existing equipment operation. In addition to EVOP, some investigators have successfully applied other advanced statistical methods to the dynamic optimization of a packed gas absorber.^[7]



Jimmy Smart is Associate Professor of Chemical and Materials Engineering at the University of Kentucky. He received his BS chemical engineering degree from Texas A&M and his MS and PhD from the University of Texas at Austin, all in chemical engineering. He has over 20 years industrial experience with companies such as IBM and Ashland Chemical. His research areas include applications of membranes to purify water supplies and treatment of hazardous wastes.

The purpose of this laboratory exercise is to introduce students to the use and application of the EVOP method. . . . Not only do they acquire knowledge of how to design a scrubber, but they also learn how the interplay of various operating parameters affects the overall scrubbing performance of the device.

The purpose of this laboratory exercise is to introduce students to the use and application of the EVOP method. Using sodium hydroxide solutions to scrub CO₂ emissions is not commonly found in industry—aqueous solutions of potassium hydroxide or amines, in conjunction with arsenite catalysts, are usually more desirable from an economic standpoint.^[8] Sodium hydroxide solutions were selected for this exercise, however, because of their ready availability in educational laboratories.

In this exercise, students are presented with a packed scrubber that is currently being used to remove CO₂ from a simulated industrial stack gas. Gas flow rate, CO₂ inlet concentration, and column diameter are fixed operational parameters. Existing conditions include use of once-through ambient water flowing countercurrent to the gas flow in a column packed with spherical packing material. Students use principles of EVOP to optimize column performance by selecting appropriate column packing, liquid recirculation rate, caustic concentration, and temperature. Column performance in this exercise is defined as lowest CO₂ emission, not lowest cost.

EVOP METHOD

Since EVOP's introduction in the late 1950s, many books and journal articles have been published discussing the method. This article is not intended as a survey review of EVOP; the reader is invited to consult the original publication or other excellent discussions^[9-12] for detailed information and its applications. The purpose of this article is to introduce undergraduate students in the chemical engineering laboratory curriculum to EVOP and to provide a procedure and list of equipment for faculty who might wish to set up a similar experiment. This introductory EVOP exercise provides a basis for further study leading to response surface theory and culminating in contemporary quality strategies in a manufacturing plant environment, such as Total Quality Management^[13] and Six Sigma.^[14]

In a research laboratory environment, strict requirements for formulating strategies of experiments can usually be satisfied. Usually, all independent and dependent variables can either be measured or carefully controlled. Principles behind orthogonal design, generation of response surfaces, randomization, experimental replication, and factorial designs can be successfully met. In a manufacturing plant environment, however, there are forces at work not subject to

control by operating personnel, including economic factors, product demands, and other undefined influences. Quite often, orthogonal designs are not compatible with production requirements.

EVOP is a procedure designed to meet the needed flexibilities inherent to the plant environment. It should be emphasized that EVOP is a routine method for permanent process operation, not an experimental procedure. It is to be applied in an existing plant operation rather than used at the pilot/laboratory scale. It was developed to avoid undesirable characteristics of full-scale process experiments that require specially trained personnel and the subsequent production of off-specification product. EVOP requires no special staff and can be used by existing plant operators after a brief training period.

Plant operators find EVOP appealing because of its intuitive approach. EVOP philosophy says to explore the effects of process variables near current operating conditions and make adjustments that will drive the process in a direction that offers improvement, whether it be quality, reduced cost, greater output, or less waste. Another added bonus behind implementation of EVOP is that it improves overall understanding of the process itself. Plant personnel gain a better understanding of the effects of process variables upon product quality. Also, subtle effects are often discovered that were not previously known to exist.

IMPLEMENTATION

The basic idea behind using EVOP is to improve the signal-to-noise ratio of an existing process in an effort to uncover relationships between operating variables. The signal is *increased* by deliberately introducing carefully chosen minor variations about an existing operational point, called the "works process." Noise within the process arises from a variety of sources, such as variability of raw materials, inability to precisely control process inputs, and instrument and measurement error. The final variation in the product yield is a composite of all these sources. The magnitude of the variation is measured by the standard deviation.

The first step in implementing EVOP is to identify pertinent process variables associated with an existing process. Then, a cycle of process runs is designed around the normal or existing values of the process variables. We deliberately introduce small changes in the process signal or process out-

puts and investigate their effects. Differences between normal and proposed values are kept necessarily small to avoid production of off-specification product. Generally, it is impractical to investigate the effects of more than three variables in an industrial process, so a 2^3 factorial design is arranged. It investigates the effects (response) of low and high levels of three process variables. Cycles of runs are repeated to replicate operational conditions and to reduce experimental error. Here, we reduce the noise level in the process by repeatedly measuring the process output at a fixed set of operating conditions.

Assume a 2^3 factorial design is set up around our first phase (ambient temperature), where the variables to be studied are recirculation rate, caustic concentration, and packing material. A "phase" is defined as a set of variables to be tested, and it forms the cubic geometry of the 2^3 factorial design, as shown in Figure 1. One complete "cycle" is defined as a complete collection of process runs from point 1 to point 8 of the cube (phase). Anywhere from three to six cycles are run for each phase to provide a valid statistical analysis. The output response to be optimized is the % CO_2 concentration in the stack gas. From Table 1, the experimental runs are set up to explore the low and high variations of these variables and the output responses for each set of conditions are noted at each apex of the cube shown in Figure 1.

Once a factorial design is arranged, it is normal statistical practice to randomize the order of the runs within each cycle. Randomization ensures that if systematic trends occur from untested variables, these effects will not be mistaken for effects from deliberately introduced changes in tested variables. Randomization also validates our analysis that assumes that errors within cycles are independent of each other. In an actual plant manufacturing environment, it is difficult to organize a random-run sequence, but by following different run sequences over the course of various cycles, randomization is assured.

After four cycles are completed for phase one, the results are averaged for each variable effect (actual results are shown in Table 1). The main effects and interaction between effects are determined from using the averages at each apex of the cube shown in Figure 1.

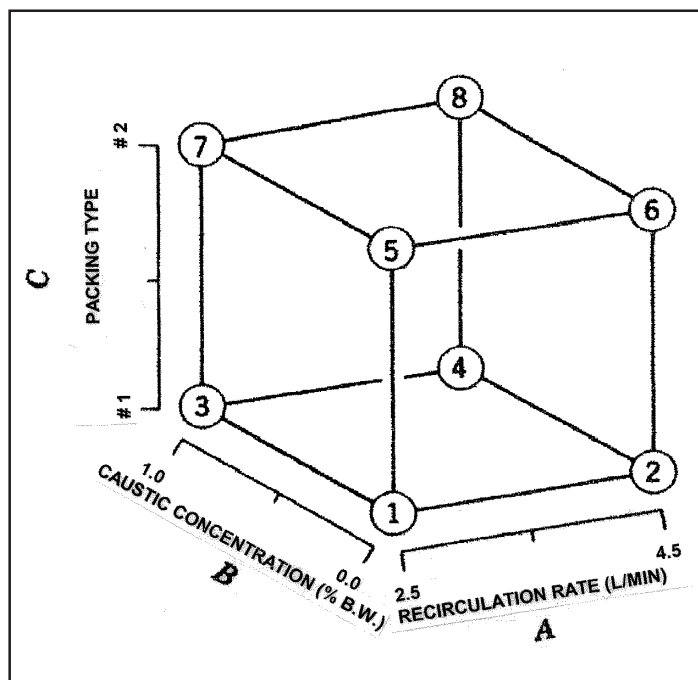


Figure 1. 2^3 factorial design for phase one.

TABLE 1
Eight Sets of Conditions of a 2^3 Factorial Design
(Phase 1 containing 4 cycles)

Run	A Recirculation Rate/ L/min	B Caustic Concentration % by wt	C Packing Type	Average CO_2 in Stack Gas % by volume
1	2.5	0.0	#1	9.87
2	4.5	0.0	#1	8.97
3	2.5	1.0	#1	7.45
4	4.5	1.0	#1	7.28
5	2.5	0.0	#2	9.90
6	4.5	0.0	#2	9.93
7	2.5	1.0	#2	6.10
8	4.5	1.0	#2	5.18

TABLE 2
Analysis of Main Effects and Interactions

		A	B	C	AB	AC	BC	ABC	± 2 S.E.
	std. mean	recirc/ dev. temp	caustic	packing					
Phase 1	8.09	1.77	-0.49	-3.17	-0.62	-0.06	-1.11	-0.42	± 1.25
Phase 2	4.64	1.53	-3.31	-2.11	1.56	-0.33	-0.60	-0.26	± 1.08

Main effects are calculated as

$$\begin{aligned} A &= \frac{1}{4}(\bar{y}_2 + \bar{y}_4 + \bar{y}_6 + \bar{y}_8) - \frac{1}{4}(\bar{y}_1 + \bar{y}_3 + \bar{y}_5 + \bar{y}_7) \\ B &= \frac{1}{4}(\bar{y}_3 + \bar{y}_4 + \bar{y}_7 + \bar{y}_8) - \frac{1}{4}(\bar{y}_1 + \bar{y}_2 + \bar{y}_5 + \bar{y}_6) \\ C &= \frac{1}{4}(\bar{y}_5 + \bar{y}_6 + \bar{y}_7 + \bar{y}_8) - \frac{1}{4}(\bar{y}_1 + \bar{y}_2 + \bar{y}_3 + \bar{y}_4) \end{aligned} \quad (1)$$

Two-factor interactions are calculated as

$$\begin{aligned} AB &= \frac{1}{4}(\bar{y}_1 + \bar{y}_4 + \bar{y}_5 + \bar{y}_8) - \frac{1}{4}(\bar{y}_2 + \bar{y}_3 + \bar{y}_6 + \bar{y}_7) \\ AC &= \frac{1}{4}(\bar{y}_1 + \bar{y}_3 + \bar{y}_6 + \bar{y}_8) - \frac{1}{4}(\bar{y}_2 + \bar{y}_4 + \bar{y}_5 + \bar{y}_7) \\ BC &= \frac{1}{4}(\bar{y}_1 + \bar{y}_2 + \bar{y}_7 + \bar{y}_8) - \frac{1}{4}(\bar{y}_3 + \bar{y}_4 + \bar{y}_5 + \bar{y}_6) \end{aligned} \quad (2)$$

Three-factor interaction is calculated as

$$ABC = \frac{1}{4}(\bar{y}_2 + \bar{y}_3 + \bar{y}_5 + \bar{y}_8) - \frac{1}{4}(\bar{y}_1 + \bar{y}_4 + \bar{y}_6 + \bar{y}_7) \quad (3)$$

Results from these calculations are summarized in Table 2. A negative sign on the main effect or interaction is desirable in this exercise because it indicates a reduction in %

CO₂ stack gas emissions.

After main effects and interactions have been tabulated, we must use a statistical tool to help us decide what variable effect is significant, *i.e.*, what response is above the “noise level” of the process. Traditional statistical tests are not appropriate in assessing the uncertainties associated with EVOP because of the small number of observations. Instead, the most practical way to evaluate EVOP uncertainty has been found to be the use of two standard-error limits. A standard error (S.E.) is the estimated standard deviation of the variable of interest. If the true standard deviation, σ , of the process variable was known, ± 2 S.E. limits would represent approximately a 95% confidence limit. The *true* standard deviation is not known, but an estimate of the standard deviation, s , can be calculated. We use this estimate to formulate our ± 2 S.E. limits to guide us in interpreting what effects and interactions are significant. Variances and standard errors can be calculated from Table 3.^[1] An estimate of the true variance, σ^2 , is calculated as

$$s^2 = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n - 1} \quad (4)$$

where s^2 is an estimate of the true variance, y_i is an individual observation, \bar{y} is the mean, and n is the total number of ob-

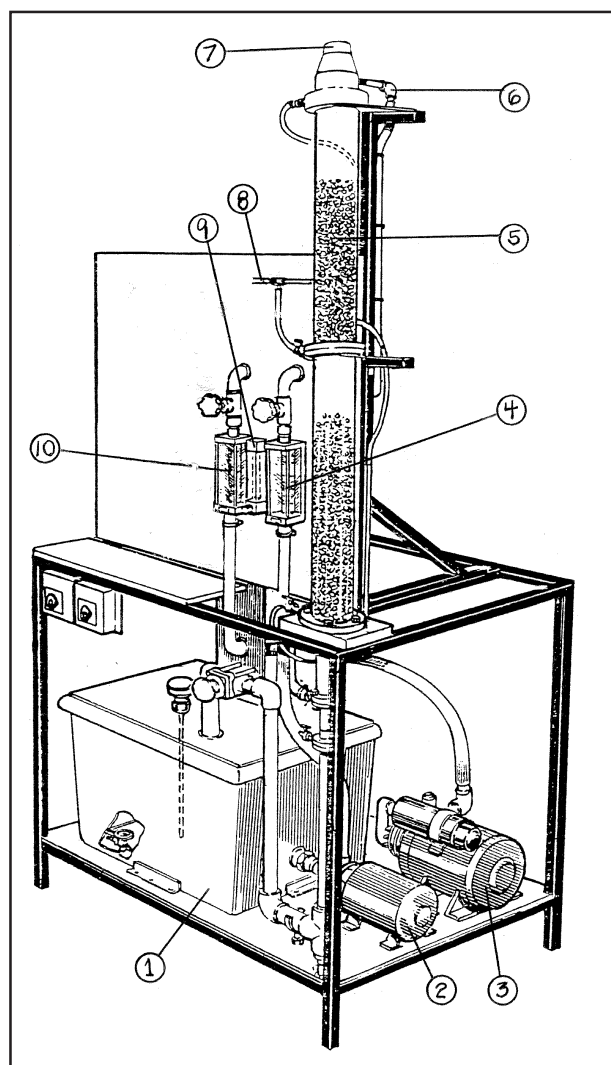


TABLE 3
Variances (σ^2) and Standard Errors for Main Effects and Interactions Estimated from a 2^p Factorial Design after c Cycles with Estimate of the Standard Deviation, s .

Design	2^p	2^2	2^3
Variance	$4\sigma^2/c2^p$	σ^2/c	$\sigma^2/2c$
Standard Error	$2s/(c2^p)^{1/2}$	$s/c^{1/2}$	$s/(2c)^{1/2}$

Figure 2.

Gas Absorption Column

Legend:

1. Recirculation sump (40-L capacity)
2. Liquid recirculation pump
3. Air blower
4. Rotameter for recirculated liquid (1-10 L/min)
5. Packing material (clear plastic column)
6. Scrubber liquor inlet
7. Scrubber discharge stack (gas outlet)
8. Pressure taps for checking Δp across the packed column
9. Rotameter for CO₂ (0-20 L/min)
10. Rotameter for air (20-180 L/min)

servations. An estimate of the true standard deviation is just $\sqrt{s^2}$. For a 2^3 factorial design, the standard error of effects is calculated as $s/\sqrt{2c}$. Therefore, the 2 S.E. limits for the effects in our design are provided by

$$\text{effect} \pm 2 \left(\frac{s}{\sqrt{2c}} \right) \quad (5)$$

Final calculated results for standard error limits are shown in Table 2. Data collected from phase two of this exercise where temperature, caustic concentration, and packing material were evaluated, are shown in Table 4.

NOTE: In the interest of reducing student laboratory time to a reasonable period, the EVOP method in this laboratory exercise has not been strictly followed in that

- Larger ranges of temperature ($\pm 13^\circ\text{C}$) were selected to clearly demonstrate their effect on scrubbing efficiency. In a plant environment, smaller temperature ranges ($\pm 5^\circ\text{C}$) would probably be selected for each factorial design (phase). Remember that one of the advantages of the EVOP method is the generation of minimal quantities of off-spec product.
- In a plant environment, four cycles would typically be used to average the output response. Instead of cycling through all eight apexes of the factorial cube before beginning the second cycle, four distinct samples for each given set of experimental conditions were collected.
- The run order was not strictly followed. For example, in phase one, in order to delay use of caustic, we followed the run order of 1-2-5-6-3-4-7-8.

EXPERIMENTAL SET-UP

An existing experimental laboratory scrubber package by Armfield, Ltd., (see Figure 2) was modified for this exercise. The column is made of clear plastic with dimensions of 9 cm OD by 1.7 m tall. The overall column consists of two packed

sections, each having a packed bed depth of 55 cm and one liquid redistributor. Three types of packing were offered to students for optimization purposes: 1/2" (1.3 cm) diameter polypropylene balls, 3/8" (1 cm) glass Pall rings, and 3/16" (0.5 cm) Jaeger stainless steel slotted rings (see Figure 3 and Table 5).

During operation of the scrubber, CO_2 is supplied from a standard gas cylinder, regulated through a rotameter, and mixed with air from an air blower to provide a 10% by volume mixture of CO_2 in air (compare this to CO_2 emissions from coal-fired power plants that are typically 14%). This gas mixture is routed to the bottom of the packed column and allowed to flow upward through the column. Scrubber liquor enters the top of the column and flows downward through the packed bed where it acts to absorb (scrub) CO_2 from the gas stream. "Clean" gas exits through the top of the scrubber. The purpose of this exercise is to find the combination of operating parameters to minimize the percent CO_2 leaving the scrubber stack.

An inexpensive (\$350) Bacharach Fyrite[®] gas analyzer was

TABLE 4
Eight Sets of Conditions of a 2^3 Factorial Design
(Phase 2 containing 4 cycles)

Run	A Temperature °C	B Caustic Concentration % by wt	C Packing Type	\bar{y} , Avg. CO_2 in Stack Gas % by volume
1	12	1.0	#2	5.05
2	38	1.0	#2	4.53
3	12	2.0	#2	3.30
4	38	2.0	#2	2.58
5	12	1.0	#3	7.25
6	38	1.0	#3	5.98
7	12	2.0	#3	5.43
8	38	2.0	#3	3.05

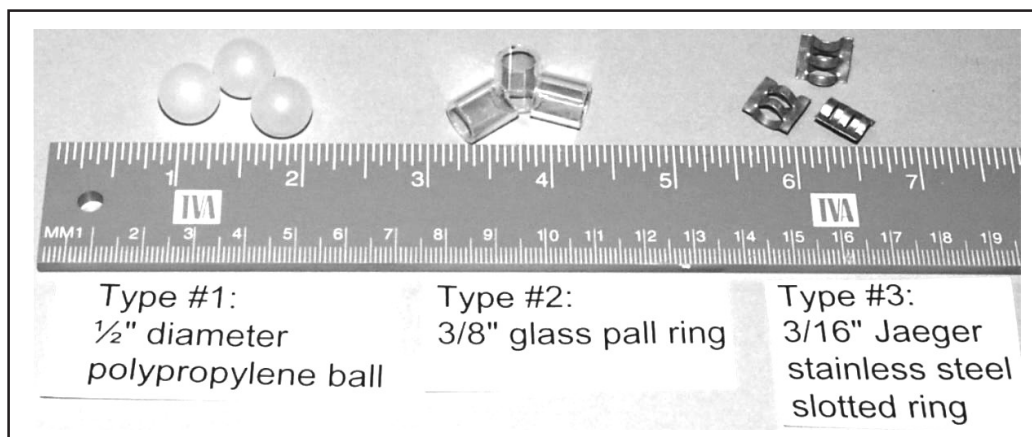


Figure 3. Random packing used for scrubber internals.

used to measure CO₂ concentrations in air for both scrubber inlet and exit. Other, more expensive, gas analyzers and analytical equipment provide greater accuracy, but ± 0.1 vol % was adequate for the purposes of this exercise. Precision, or repeatability, under experimental conditions proved to be $\pm 8\%$. The Fyrite provides a quick and easy method for measurement of CO₂ in air. It employs the Orsat method of volumetric analysis involving chemical absorption of carbon dioxide into a potassium hydroxide solution. A rubber bulb is used to draw the gas sample into the indicator solution. The instrument is inverted and the percentage of gas absorbed by the Fyrite fluid is immediately read from the scale (0-20%). Temperature of the scrubber recirculation sump was controlled by a bath circulator (NESLAB Instruments, RTE-100) fitted with an external cooling coil.

Teams of three to five students can be formed to complete this exercise. Safety procedures should include familiarity with the NaOH Material Safety Data Sheet (MSDS) and Fyrite device, location of the eyewash/shower, and wearing appropriate personal protective equipment (PPE) for handling caus-

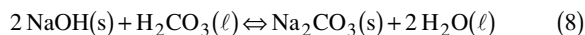
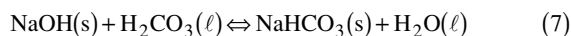
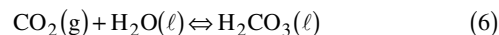
tic. The first set of data (varying concentration at ambient temperature) can be collected in one afternoon, but the more lengthy elevated/reduced temperature settings require completion on subsequent days.

After students become familiar with the equipment and have characterized existing scrubber performance, they are ready to apply the EVOP method. A 2³ factorial experimental matrix is set up to measure the response (level of CO₂ emissions) from small changes in operating variables (liquid flow rate, caustic concentration, and temperature). Standard error limits are tabulated to build response surfaces to judge positive and negative effects of parameter changes for a given packing material. Results from these small changes are used to guide the students in making judgments as to what direction parameters should be adjusted to achieve a final process optimum.

The final submitted report should include safety and operational procedures, collected data, calculations, results, sources of experimental error, and a discussion that includes which direction the final process optimum will lie and how to proceed to locate this optimum.

DISCUSSION

In actual scrubbers at industrial power plants, Ca(OH)₂, called slaked lime, is used to remove the hazardous air pollutant, sulfur dioxide, from stack gases. In this experiment, another strong base, NaOH, is used to remove CO₂ from our simulated stack gas. The primary reactions that occur during the scrubbing process are



In Eq. (6), a weak dibasic acid, carbonic acid, is formed when carbon dioxide is mixed with water. As the caustic solution (a strong base) contacts the carbonic acid, either sodium bicarbonate is formed from Eq. (7) or sodium carbonate from Eq. (8). The reactions can be found as titration curves in any standard analytical chemistry text^[15] and can be monitored in the scrubber with a pH probe.

In the absorption process, the overall rate is governed by diffusion and chemical reactions occurring in the liquid phase. The reaction is a pseudo first-order reaction between dissolved CO₂ and OH⁻ in the liquid and is of the same order of magnitude as the rate of diffusion.^[16]

For an industrial scrubber, a tank supplying scrubber medium typically contains several thousand gallons. Unfortunately, the working volume of the small recirculation sump in our experimental apparatus is only about 38 L. Based on an assumption of plug flow at a recirculation rate of 4.5 L/min, where the pump suction and recirculated liquor return

TABLE 5
Properties of Random Packing

Packing Type	Packing pieces/cm ³	Surface area/vol Δp/L (cm water/cm (cm ² /cm ³)@ 2.5 ml liquid/min	Pressure drop:
#1: 1/2"-diameter P/P sphere	4.2	21.3	0.16
#2: 3/8" glass Pall ring	5.5	35.2	0.06
#3: 3/16: Jaeger s.s. slotted ring	18.1	49.0	0.05

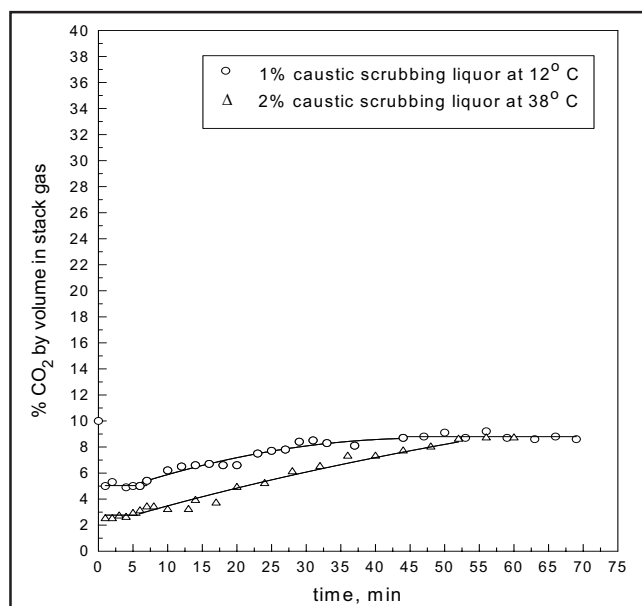


Figure 4. Unsteady-state nature of scrubber performance: recirc rate, 4.5 L/min, #2 packing (lines added to guide the eye).

are located at opposite ends of the sump, a working time of only 8.5 minutes is available. The unsteady-state nature of the scrubbing action is charted in Figure 4. Sure enough, for about 8 minutes, the percent CO_2 by volume in air is 5.0. After this period, the percent CO_2 slowly climbs to a steady-state value of 8.8 after 44 minutes. During the initial 8 minutes, the sodium carbonate salt (Eq.8) is probably being formed. After the initial period there are probably equilibrium competitions between Eqs. (7) and (8), until a steady-state condition is attained.

As previously mentioned, repeatability of experimental measurements with the gas analyzer was $\pm 8\%$. This value would be viewed as high in a laboratory setting, but is probably a realistic value in a plant environment. The lack of repeatability was not due to the instrument itself, but was primarily due to gas-flow drifting fluctuations in the rotameter, Joule-Thompson effects of gas expansion across the CO_2 cylinder regulator, and observed channeling effects of liquid flow in the packed column.

RESULTS

The main effects and interactions between process variables are summarized in Table 2. In phase 1, recirculation rate (A), % caustic (B), and packing material (C) were evaluated. From consideration of each effect ± 2 S.E., it appears the increase of caustic from 0% to 1% had a strong negative effect (decreasing the percent of CO_2 in the stack gas, which is a desirable outcome). The other effects are not significant since they are below the error limits and can be considered to be within the noise of the process. One surprising result is the fact that the main effect (A) of the recirculation rate was not significant. There was no advantage to increasing the recirculation rate from 2.5 to 4.5 L/min. Evidently, the scrubbing effect is not diffusion-rate limited, but reaction-rate limited.

In phase 2 of Table 2, the temperature (A), % caustic (B), and packing material (C) were evaluated. From consideration of each effect ± 2 S.E., it appears only the main effects of temperature (A), % caustic (B), and packing material (C) were significant. The result of increasing the temperature and % caustic had a strong negative effect (decreasing the % CO_2 in the stack gas). On the other hand, switching the packing from Pall rings to more open stainless steel slotted rings had a strong positive effect (increasing the % CO_2 in the stack gas). This is a somewhat surprising result, since the slotted rings offer more surface area/volume and less pressure drop (see Table 5). This can be explained (as was shown from results of phase 1) by the fact that the scrubbing effect is limited by reaction rate, not the diffusion rate. The slotted rings offer more open geometry (less Δp) and therefore less liquid holdup within the packed beds. With glass Pall rings, there is more liquid holdup within the column, which favors reaction between CO_2 to form the carbonates. In the case of packing #1 (P/P spheres), this geometry offers a much reduced surface area/volume,

which lowers the reaction rate between the gas and liquid phases within the column.

CONCLUSIONS

From this abbreviated application of EVOP, we can draw some conclusions as to what direction the optimum for this scrubbing process might lie. The optimum will reside in a direction of elevated operating temperature and higher % caustic in the scrubbing liquor. Packing material #2 (Pall rings) is more desirable in decreasing the overall % CO_2 in the stack gas, but is just slightly out of the error limits. In the final analysis, packing #3 (slotted rings) may be a more favorable choice because of the lower operating cost (less Δp /length of packing height).

From the EVOP analysis, use of higher % caustic reduced CO_2 emissions from our scrubber stack. Where might the overall process optimum reside? From the MSDS, sodium bicarbonate is soluble in water to about 8% b.w. at 18°C . Therefore, this condition would be the limiting factor on what maximum concentration of NaOH to use in the scrubbing liquor. Anything above about 8% to 10% would cause salting-out of solids that would foul and possibly occlude scrubber packing. It is interesting to compare the main effect of % caustic for phase 1 and phase 2. Moving from 0% caustic to 1% had a very strong negative effect (CO_2 reduced in stack gas), whereas moving from 1% to 2% had a less strong negative effect. The response surface is not linear. This situation calls for additional investigation, as a process optimum may reside somewhere between 2% caustic and the recommended maximum limit of 10% caustic. Other investigators^[17] have found the optimum mass transfer coefficient to reside at a 2M NaOH solution (about 8% b.w.).

Where might the elevated process optimum temperature lie? A cost analysis would have to be performed on a better-defined response surface to identify optimum temperature. In a plant environment, unless low-pressure waste steam is available, the energy costs to heat the scrubber liquor is probably not justified. One point to consider, however, is that usually inlet stack gases fed to scrubbers (especially those from power plants) are often at elevated temperatures. Another alternative is to add 50% b.w. caustic with enough water in a mixing tee to form a 10% b.w. caustic solution just prior to its introduction to the scrubber. This method would allow some elevation of temperature due to heat of solution.

This exercise has been prepared to provide an undergraduate student with experience in the use and application of the EVOP method in a laboratory environment. As demonstrated, the student can set up additional variable ranges to be tested for phases 3 and 4, and so forth, to identify a final optimization of the overall scrubbing process.

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Book Review: *Discussion of the Method*

Continued from page 203.

did not wish to appeal to Greek authority. Readers must either accept Koen's synopsis of such major thinkers as Kant, Gödel, and Wittgenstein, or they must be conversant with the history of Western thought, principally in philosophy. This requires either an abstraction of the thinkers cited, or many years of reading.

William Perry^[2] suggested that the intellectual development of college students consists of stages that progress from authoritarian dualism (Stages 1 through 3) through the slough of relativism (Stages 4 through 6) to committed action (Stages 7 through 9), and indicated that relativism is where many college students get stuck. The relative equality of opinion and the absence of authority lead to the lack of commitment that is sometimes predominant in education today.

As applied to pedagogy, Koen's book also suggests that a departure from authority (dualism) is good, but going beyond relativism is better. Koen's method for doing so is through heuristics. Heuristics, or general rules-of-thumb, are particularly important guides in the absence of absolutes.

Koen's book provides some guidance in dealing with ambivalence of contrasting heuristics, often incorporated in society's aphorisms. How does one balance the contrasting heuristics of "Look before you leap," with "He who hesitates is lost"? It is clear that the triage advice, "When you hear hoofbeats, think horses not zebras," has a geographic limitation—it applies more in the Western world than Africa. According to Koen, contradictions require judgment to obtain a basis for action, to get beyond relativism.

In the score of years since its original publication, Koen's ASEE book has been used in a freshman honors seminar "Paradoxes of the Human Condition," with between 12 and

15 students per year, in an effort to find a way beyond Relativism in the Absolute versus Relative paradox. One week the students discuss the Absolute through Descartes' effort to break from Greek authority. The following week the students discuss Koen's *Definition of the Engineering Method* in parallel with Perry's model of intellectual development.

Our students' essays indicate that a study of Koen's heuristics initiates progress away from a Relativistic position. In other words, even though an absolute is not known, heuristics show the way to take appropriate action, or to choose between two actions. As such, the students readily embrace Koen's perspective of heuristics, and their combination into a state-of-the-art, or paradigm.

Professor Koen's book suggests a startling, explicit statement of a new way to think about engineering and life, but a method which may already be implicit in the subconscious of most practicing engineers. If we, as educators, wish to prepare our students for engineering practice, the techniques indicated in this book provide a philosophical underpinning for dealing with risks associated with engineering actions and designs, when there is insufficient applicable science. The interesting extension of Koen's engineering philosophy to life is, at a minimum, worthy of our consideration.

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A QUADRUPLE-TANK PROCESS CONTROL EXPERIMENT

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While analytical calculations and process simulations^[1,2] should be a key component in the education of a chemical engineer, students gain a deeper understanding of the nonidealities of industrial processes by carrying out experiments. Many industrial control problems are nonlinear and have multiple manipulated and controlled variables. It is common for models of industrial processes to have significant uncertainties, strong interactions, and/or non-minimum phase behavior (*i.e.*, right-half-plane transmission zeros). Chemical engineering students especially find the concept of right-half-plane transmission zeros to be more subtle than other concepts.

We designed a quadruple-tank process that was constructed to give undergraduate chemical engineers laboratory experience with key multivariable control concepts (see Fig. 1). By changing two flow ratios in the apparatus, a range of multivariable interactions can be investigated by using only the one experimental apparatus. Since the spring of 1999, this quadruple tank process has been used to teach students at the University of Illinois to

- Understand control limitations due to interactions, model uncertainties, non-minimum phase behavior, and unpredictable time variations
- Design decentralized (often called “multiloop”) controllers, and understand their limitations
- Implement decouplers to reduce the effect of interactions, and understand their limitations
- Implement a fully multivariable control system
- Select the best control structure, based on the characteristics of the multivariable process

The quadruple-tank apparatus is a variation on an apparatus described in the literature^[3] where we introduced a time-varying interaction between the tanks. This time-varying characteristic is caused by an irregularity in the fluid mechanics of splitting the stream into the upper and lower tanks, which results from the capillary effect of the tubing and dynamics

of the multiphase flow of liquid and air in the tubing. The consequence of combining these factors is an enhanced sensitivity and stochasticity of the flow ratio to manipulated variable movements. The apparatus can exhibit a time-varying qualitative change in its dynamics, between conditions that are controllable to those that are uncontrollable. Although this uncontrollability issue has been reported as a major issue in large-scale industrial processes,^[4] this appears to be the first educational laboratory experiment designed to clearly illustrate it and its effects on the control system.

The apparatus is small (1 ft x 1 ft x 6 in, not counting computer equipment) and is designed so the students, teaching assistants, and instructor can determine at a glance if the students are controlling the apparatus successfully. The small size enables experimental data to be collected rapidly and keeps the cost low. The apparatus is designed to be self-contained (that is, there are no requirements for continual access to water, steam, vacuum, or gas) and is environmentally friendly—the only chemical used is ordinary tap water, which is recycled during the experiments.

Past studies with 4-tank apparatuses implemented decentralized PI control,^[3] multivariable H_∞ control,^[3] multivariable internal model control,^[5] and dynamic matrix control.^[5]

Siong Ang received his BS in chemical engineering from the University of Illinois under a Singapore Armed Forces Overseas Merit Scholarship and his MS from Stanford University. As part of his undergraduate thesis, he constructed quadruple-tank-process experiments and wrote the visual-programming control interface currently used in the undergraduate process control laboratory.

Effendi Rusli received his BS from the University of Wisconsin and his MS from the University of Illinois at Urbana-Champaign, both in chemical engineering. He is currently completing his PhD thesis on the analysis and control of systems described by multiscale simulation codes, with the main application being the electrodeposition of copper films and wires in microelectronic devices.

Richard Braatz received his BS from Oregon State University and his MS and PhD from the California Institute of Technology. After a postdoctoral year at DuPont, he joined the faculty at the University of Illinois, where he is a Professor and University Scholar. His main research interest is in multiscale systems theory and its application. He has published three books, one of which is a textbook on fault detection and diagnosis.

The main educational focus of Ref. 3 was providing an apparatus with highly idealized and reproducible dynamics for use in illustrating multivariable interactions and multivariable transmission zeros. The main educational focus of Ref. 5 was to provide hands-on experience for students in implementing advanced control algorithms. In contrast, *our main educational focus is to aid students in understanding the advantages and disadvantages of the different control structures (e.g., decentralized, decoupling, multivariable) when applied to a multivariable process with interactions and dynamics ranging from highly ideal to highly nonideal.*

First, the construction of the apparatus will be described here in enough detail for duplication. Enough information will be provided for a technician or student to construct the control apparatus and for an instructor (who may not be an expert in control) to see how to use the experiment in the laboratory. This will be followed by motivation and background on the modeling and control for the apparatus. Some experimental results obtained by two students will also be presented to show how the apparatus illustrates some key control principles that are not addressed by past control experiments.

EXPERIMENTAL APPARATUS

A table of all equipment needed to construct the apparatus, including costs, can be obtained from the website at <<http://brahms.scs.uiuc.edu>>. Four cylindrical tanks are mounted vertically on an acrylic board and are arranged in a symmetric 2 x 2 fashion, as shown in Figure 1. A small hole is drilled at the bottom of each tank to channel the water from each to a

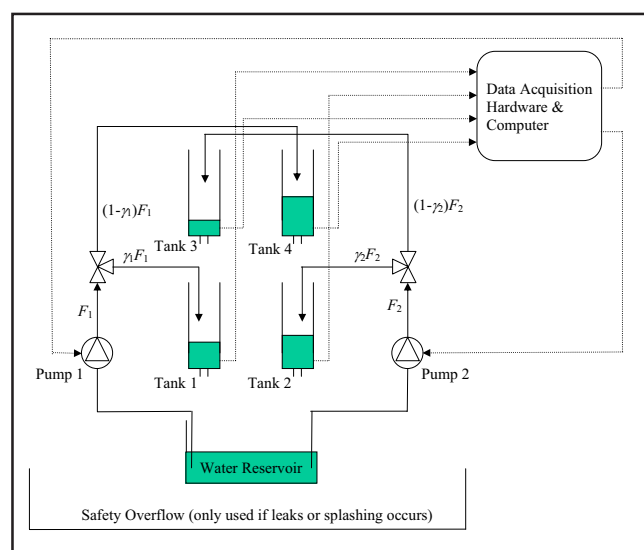


Figure 1. Schematic of the quadruple-tank process apparatus. To simplify the figure, not shown are a tube between Tank 3 and Tank 1, a tube between Tank 4 and Tank 2, a tube from Tank 1 to the water reservoir, a tube between Tank 2 and the water reservoir, and a lid on the water reservoir. These tubes and lid are used to reduce evaporation.

differential pressure sensor via a 3/16-in tubing. MASTERFLEX tubings transport water between the tanks. Taking into account the maximum capacity of all four tanks (750 ml) and the dead volume inside the entire length of the tubings, a 1000-ml cylindrical beaker is enough to store and recycle water for the experiments. Two MASTERFLEX volumetric pumps are used. A 5-gallon tank immediately below the apparatus contains any spillage or splashing from overflow in any of the four tanks.

A Y-junction is used to divide the flow such that water is channeled to a bottom-level tank and the upper-level tank diagonal to it. This arrangement makes both levels in the bottom two tanks a function of both pump-flow rates. By adjusting the valve knob, the process can be operated so that one of the multivariable transition zeros is in the right-half plane, the left-half plane, or switches between the two planes in a stochastic time-varying manner.

The low cross-sectional area of the tanks makes level variations easy to see with the naked eye. Hence, students, teaching assistants, and instructors can assess the performance of the closed-loop system with a glance. The tank heights are small, so the closed-loop controllers that perform poorly lead to overflow in the tanks, which is an indication that the control system needs either better tuning or an alternative control structure, or the interactions need to be changed to make the process more controllable.

The visual programming control interface used in the laboratory^[6] was modified for use with this apparatus. It enables students with a minimum background in computer programming to make changes in the control structures and is available for download at a web site.^[7] Readers can find more details in the references.

MOTIVATION FOR THE APPARATUS

There are several advantages to including a quadruple-tank process experiment in an undergraduate chemical engineering laboratory. One is that the experiment can demonstrate a range of interactions from slight to very strong. The apparatus allows students to investigate the extent to which a decentralized controller is capable of controlling the process as the interactions increase. They can also implement partial or full decoupling as a first step to reduce process interactions. This enables students to obtain hands-on experience in how decoupling can improve the closed-loop performance in some situations (when there are some interactions, but not too strong), while having significant limitations when the interactions become sufficiently strong.^[8]

The quadruple-tank dynamics have an adjustable multivariable transition zero, whose position can be in the left- or the right-half plane, depending on the ratio of flow rates between the tanks. This enables students to investigate performance limitations due to right-half-plane transmission zeros. For the particular quadruple-tank apparatus at the University of Illi-

nois, under certain conditions the transmission zero can move between the left- and right-half planes, with varying levels of stochasticity depending on the operating condition. This leads to some interesting time-varying dynamics.

BACKGROUND

The experimental apparatus is used to teach important principles of process control while familiarizing chemical engineers with control structures used in industry. In the laboratory reports, students describe each learned control principle in words and illustrate the principle for the quadruple-tank process by first-principles modeling, applying control theory learned in lecture, and experimental verification. This draws a close connection between what the students learn in the lecture and what they practice in the laboratory.

The material balance equations using common assumptions and the transfer function matrix obtained by linearizing and taking deviation variables are given in Figure 2. The second-order transfer functions correspond to the contributions to the bottom two tanks by the upper two tanks. The linearized system $G(s)$ in Figure 2 has two multivariable transmission zeros, which are determined by the zeros of its determinant

$$\det G(s) = \frac{c_1 c_2 \gamma_1 \gamma_2}{\prod_{i=1}^4 (1 + sT_i)} \left[(1 + sT_3)(1 + sT_4) - \frac{(1 - \gamma_1)(1 - \gamma_2)}{\gamma_1 \gamma_2} \right] \quad (1)$$

It is important to determine the location of these zeros in the complex plane since right-half-plane zeros limit the closed-loop performance achievable by any control system.^[8,9] For the sake of convenience, the parameter η is introduced as

$$\eta = \frac{(1 - \gamma_1)(1 - \gamma_2)}{\gamma_1 \gamma_2} \quad (2)$$

where $\eta \in (0, \infty)$. Since the numerator of Eq. (1) is a quadratic, the zeros can be computed analytically

$$z_{1,2}(\eta) = \frac{-(T_3 + T_4) \pm \sqrt{(T_3 - T_4)^2 + 4T_3 T_4 \eta}}{2T_3 T_4} \quad (3)$$

Given $T_3 > 0$ and $T_4 > 0$, the function in Eq. (3) is differentiable for $\eta \in (0, \infty)$.

$$z'_{1,2}(\eta) = \pm \frac{1}{\sqrt{(T_3 - T_4)^2 + 4T_3 T_4 \eta}} \quad (4)$$

The derivatives exist for all conditions where $T_3 \neq T_4$. When $\eta = 0$, the zeros are $z_1 = -1/T_3$ and $z_2 = -1/T_4$. As η approaches ∞ , it is straightforward to deduce from Eq. (3) that

$$z_1 \rightarrow \sqrt{\eta/T_3 T_4} \quad \text{and} \quad z_2 \rightarrow -\sqrt{\eta/T_3 T_4}$$

Because the derivative functions in Eq. (4) are monotonic, z_1 is strictly increasing and z_2 is strictly decreasing. This im-

plies that the transmission zero z_1 will cross from the left-half plane to the right-half-plane with increasing η . The crossing occurs at $\eta = 1$. With a little algebra, these results can be written in terms of the flow ratios γ_1 and γ_2 , as shown in Table 1.

The process is minimum phase when the total flow to the lower tanks is greater than the total flow to the upper tanks ($1 < \gamma_1 + \gamma_2 < 2$). The process is non-minimum phase (that is, has a multivariable transmission zero in the right-half plane) when the total flow to the lower tanks is smaller than the total flow to the upper tanks. For operating conditions where the total flow to the upper tanks is nearly the same as the total flow to the lower tanks, small variations in the flows due to irregular behavior in the tubing can cause the transmission zero to move between the two half planes in an irregular manner, in which case the process becomes uncontrollable.^[9]

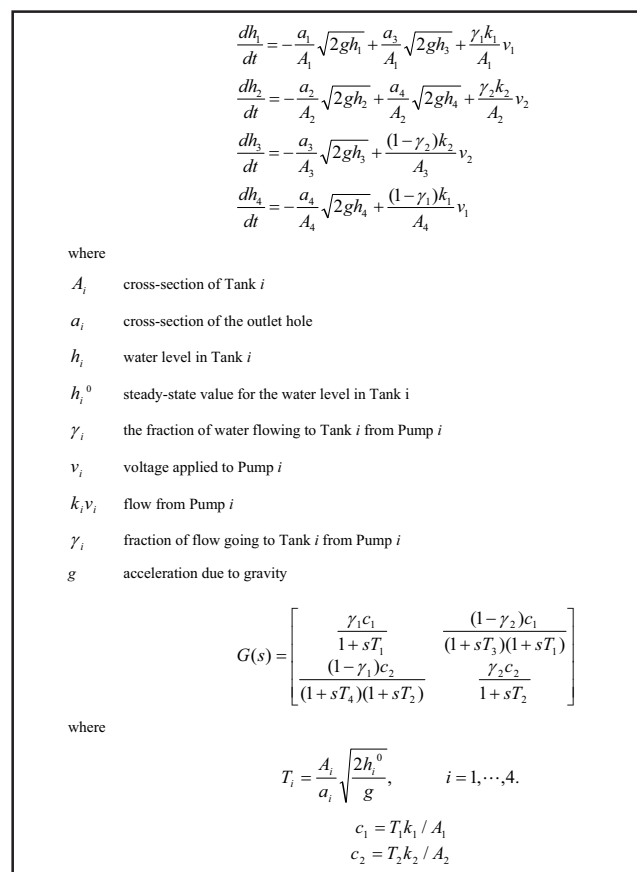


Figure 2. Physical models for quadruple-tank process.^[3]

TABLE 1
Location of Zeros on the Linearized System as a Function of the Flow Ratios γ_1 and γ_2

	z_1	z_2	
$1 < \gamma_1 + \gamma_2 \leq 2$	negative	negative	minimum phase
$\gamma_1 + \gamma_2 = 1$	zero	negative	boundary
$0 \leq \gamma_1 + \gamma_2 < 1$	positive	negative	nonminimum phase

More precisely, the steady-state determinant of the transfer function $[G(0)]$ in Figure 2] switches sign when $\gamma_1 + \gamma_2$ crosses 1, indicating that it is impossible to control the process with a linear time invariant feedback controller with integral action.^[9] This is a generalization of the single-loop notion that the sign of the steady-state gain must be either consistently positive or consistently negative for the process to be controllable with a linear feedback controller with integral action.

Students have applied decentralized control, decoupling control, and fully multivariable control on the same apparatus. They compare different multivariable control structures and judge for themselves the most effective method to control the apparatus. It is important for the students to realize that the same structure can perform very differently and they will face a new set of limitations when conditions change. This is especially relevant to this particular apparatus in which under some conditions the process becomes uncontrollable during movement of the transmission zero across the imaginary axis within a single setpoint or disturbance response.

After investigating decentralized control, decoupling is implemented as the first step to deal with loop interactions. Students verify the improvement/deterioration in closed-loop

performance caused by the implementation of decoupling. The details of the implementation vary depending on the type of decoupling (steady-state, dynamic, partial, full), but all of these are easy to implement using the control interface.^[6] Students also investigate the effects of model uncertainties, which are especially important for this apparatus.

EXAMPLE IDENTIFICATION RESULTS

The identification experiment is an ascending series of steps followed by subsequent descending steps for identification, which is a better input for characterizing process nonlinearities. The use of ascending and descending step inputs has the educational benefit of permitting visual monitoring of the change in the dynamics with different level of operating regime and checking of the reproducibility of the process response.

To ease them into the process, students are prompted to first operate the apparatus so that most of the flow goes to the bottom two tanks. The first step is to determine the transfer function matrix for the experimental apparatus for comparison to the theoretical model. Various student teams have fit first-order-plus-time-delay, state space, and ARMAX models to experimental data. For brevity, only transfer functions determined using the program *ms2th*,^[10] which is a MATLAB built-in identification subroutine, to compute the least-squares estimate of both discrete and continuous model parameters, are reported here for one operating condition:

$$y(s) = G(s)u(s) + H(s)e(s) \quad (5)$$

$$G(s) = \begin{bmatrix} \frac{11.89}{121.4s + 1} & \frac{6.875}{(121.4s + 1)(3.967s + 1)} \\ \frac{6.738}{(84.73s + 1)(3.109s + 1)} & \frac{11.53}{84.73s + 1} \end{bmatrix} \quad (6)$$

$$H(s) = \begin{bmatrix} 2.179 \frac{2.074s + 1}{121.4s + 1} & 1.529 \frac{(1.410s + 1)(7.970s + 1)}{(121.4s + 1)(3.967s + 1)} \\ 2.382 \frac{8.75s^2 + 5.75s + 1}{(3.109s + 1)(84.73s + 1)} & 1.652 \frac{2.725s + 1}{84.73s + 1} \end{bmatrix} \quad (7)$$

where $u(s)$ is the vector of voltage signals from the two pumps, $y(s)$ is the vector of heights of Tanks 1 and 2, and $H(s)$ has been normalized so that the noise signal $e(s)$ is uncorrelated with unit variance. Comparing the theoretical transfer function model in Figure 2 with Eq. 7 gives the nominal estimates of the physical parameters

$$\gamma_1 = 0.63 \quad \gamma_2 = 0.64 \quad c_1 = 18.94 \quad c_2 = 18.10$$

which would indicate that both transmission zeros are in the left-half plane (see Table 1). Figure 3 compares the predic-

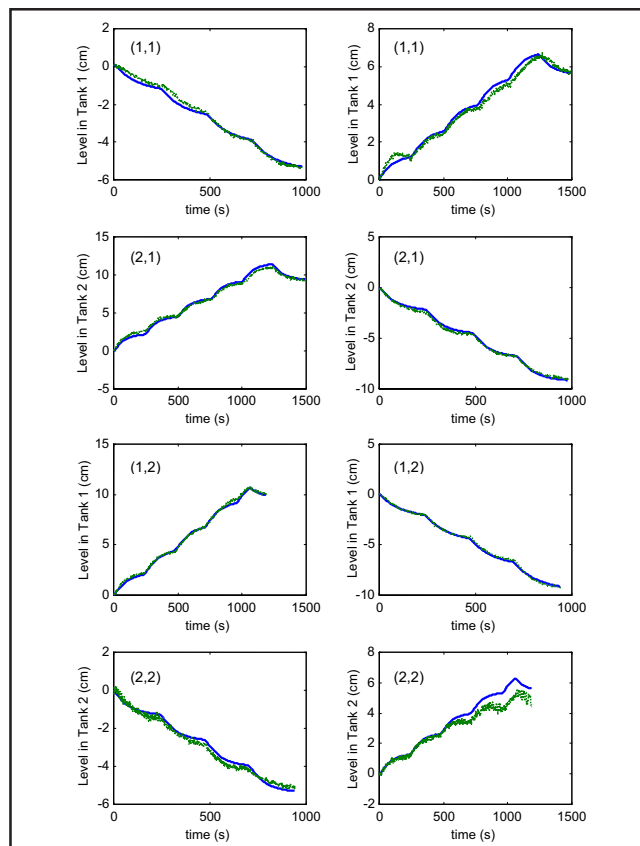


Figure 3. Model predictions plotted with experimental data for the four elements of the transfer function matrix: data used to fit model (left), data used to verify model (right). The row and column numbers are reported in the upper-left corner.

tions of the model (6) and experimental data. There is some variation in the gains, which agrees with an experimental observation that the flow ratios vary depending on the operating conditions and that the gains are a function of the flow ratios (see Figure 2). Using basic statistics,^[11] the 95% confidence intervals for the flow ratios are $0.48 < \gamma_1 < 0.79$ and $0.49 < \gamma_2 < 0.80$, which suggest that the transmission zero may move into the right-half plane under some operating conditions. This has serious implications on feedback controller design, as seen below.

EXAMPLE MULTIVARIABLE CONTROL RESULTS

Full multivariable control such as model predictive control can be implemented that manipulates the signals to the pumps to control levels in the bottom two tanks.^[5] While such multivariable controllers are being increasingly implemented in industry, other types of controllers have been applied in the chemical industries, such as

- **Decentralized control:** a noninteracting controller with single-loop controllers designed for each tank. Control loop 1 manipulates the flow through Pump 1 (via a voltage signal) to control the height of Tank 1, while Control loop 2 manipulates the flow through Pump 2 to control the height of Tank 2.
- **Partial decoupling** followed by decentralized control.
- **Full decoupling** followed by decentralized control.

Various students have implemented these control strategies on the quadruple-tank process apparatus during the past five years. Students implement up to three control strategies in a 7-week period, where the scheduled lab time is 3 hours per week and the lab report requirements include first-principles modeling, analysis, and comparison between theory and experiment.

The relative gain for the nominal plant (6) is 1.5, which indicates that Pump *i* should be paired to the level in Tank *I* (8). Decentralized Internal Model Control Proportional-Integral (ICM-PI) controllers are tuned to trade off robustness with performance^[8,9,12] (see Table 2 and Figures 4 and 5 for two levels of tuning). Due to model uncertainties, the differences between model predictions and experiments are large when the IMC-PI controllers are tuning too aggressively.

Implementing a partial dynamic decoupler and multiplying by the transfer function matrix in Figure 2 gives

$$\tilde{G}(s) = \begin{bmatrix} \frac{\gamma_1 c_1}{1 + sT_1} & 0 \\ \frac{(1 - \gamma_1)c_2}{(1 + sT_4)(1 + sT_2)} & \frac{\gamma_2 c_2 \Theta}{(1 + sT_2)(1 + sT_3)(1 + sT_4)} \end{bmatrix} \quad (8)$$

$$\Theta = (1 + sT_3)(1 + sT_4) - \frac{(1 - \gamma_1)(1 - \gamma_2)}{\gamma_1 \gamma_2}$$

TABLE 2
Proportional Gains, *K*, and Integral Time Constants, τ_I for Decentralized Controllers with Aggressive and Sluggish Tuning

		<i>K</i>	τ_I
		Aggressive	Sluggish
Aggressive	<i>C</i> ₁	1	121.4
	<i>C</i> ₂	1	84.73
Sluggish	<i>C</i> ₁	0.378	121.4
	<i>C</i> ₂	0.395	84.73

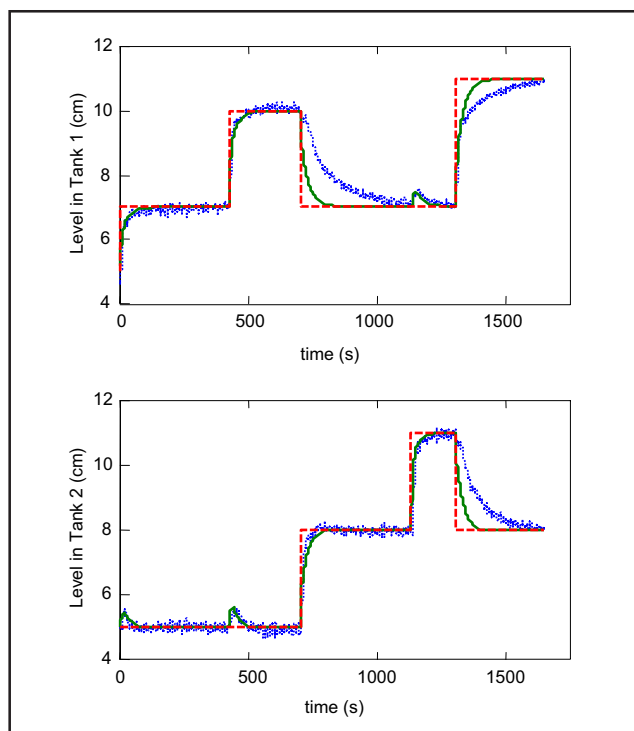


Figure 4. Decentralized controller with aggressive tuning: setpoint (dashed line), experiment (dots), model prediction (solid line).

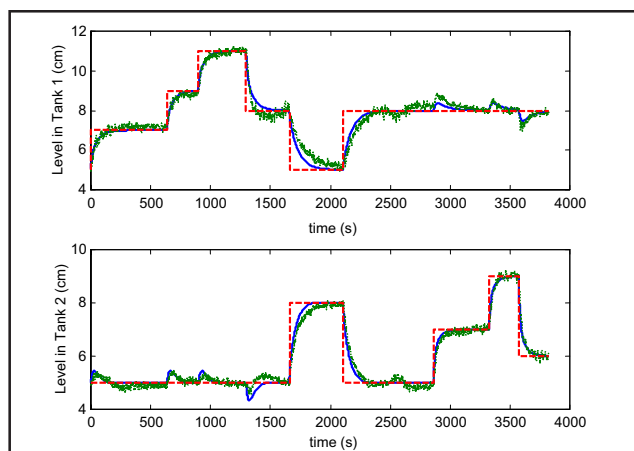


Figure 5. Decentralized controller with sluggish tuning: setpoint (dashed line), experiment (dots), model prediction (solid line).

TABLE 3
Proportional Gains, K , and Integral Time Constants, τ_I
for Partially Decoupled Controllers with Aggressive and
Sluggish Tuning

		K	τ_I
Aggressive	C_1	1	121.4
	C_2	1	84.73
Sluggish	C_1	0.3	121.4
	C_2	0.3	84.73

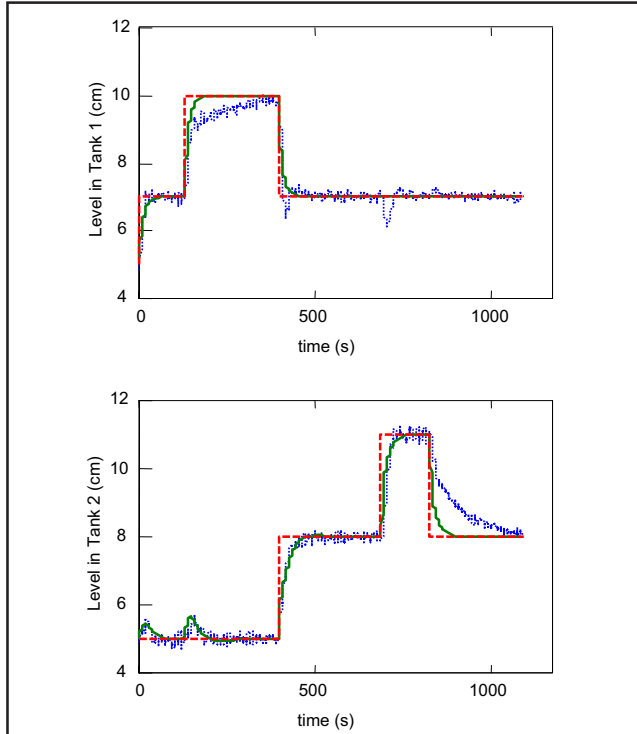


Figure 6. Partial decoupling with aggressive tuning: setpoint (dashed line), experiment (dots), model prediction (solid line).

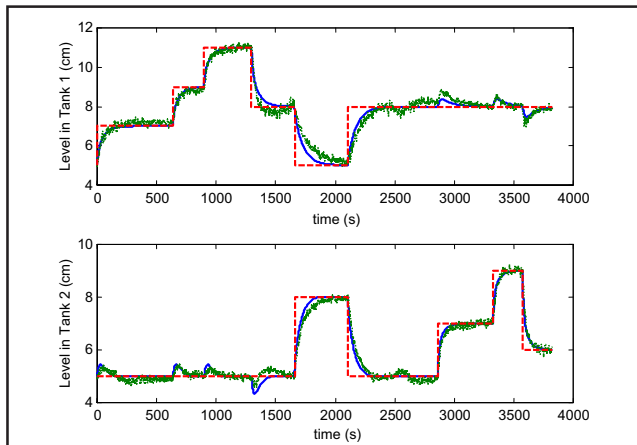


Figure 7. Partial decoupling with sluggish tuning: setpoint (dashed line), experiment (dots), model prediction (solid line).

The transmission zeros are values of s in which $\Theta = 0$ (see Eq. 5). Both transmission zeros appear in the second control loop. This results in a degradation of the closed-loop performance for the second control loop when one of these transmission zeros is in the right-half plane. Using model (6), the results of tuning IMC-PI controllers to trade off robustness with performance are shown in Table 3 and Figures 6 and 7. Both aggressive and sluggish tuning shows some interactions between the control loops, due to plant/model mismatch. The differences between the model predictions and experimental data are larger for the aggressive tuning.

While full dynamic decoupling is not common industrial practice, for educational purposes it is useful to compare full dynamic decoupling with partial dynamic decoupling to illustrate how full decoupling can lead to worse closed-loop performance than partial decoupling. Implementing a full dynamic decoupler and multiplying by the transfer function matrix in Figure 2 gives

$$\tilde{G}(s) = \begin{bmatrix} \frac{\gamma_1 c_1 \Theta}{(1+sT_1)(1+sT_3)(1+sT_4)} & 0 \\ 0 & \frac{\gamma_2 c_2 \Theta}{(1+sT_2)(1+sT_3)(1+sT_4)} \end{bmatrix} \quad (9)$$

The transmission zeros appear in both control loops. When one transmission zero is in the right-half plane, its effect on both loops implies that the closed-loop performance can be worse for full decoupling than for partial decoupling, since the right-half-plane transmission zero will affect both control loops. Using model (6), the model predictions and experimental data using the IMC-PI controllers in Table 3 are shown in Figures 8 and 9 (next page). The closed-loop responses with full decoupling are much worse than for the decentralized or partial decoupling controllers. In most cases when stepping up the setpoint, there appears to be inverse response exhibited in both control loops, suggesting that the closed-loop system is stable but a transmission zero has moved into the right-half plane. *That interpretation would be incorrect.* While it is correct that a transmission zero moves into the right-half plane when the setpoint is stepped up, the closed-loop system becomes *locally unstable* when this occurs. This is because the steady-state gains in (9) change sign, switching the controllers from negative to positive feedback. This is a common issue in large-scale industrial systems, which can be masked when physical constraints are present.^[4,13-14]

To see the change in sign, consider the entry (2,2) in the transfer function matrices (8) and (9)

$$g_1(s) = \frac{\gamma_2 c_2 \Theta(s)}{(1+sT_2)(1+sT_3)(1+sT_4)} \quad (10)$$

Since $\gamma_2 c_2 > 0$, the sign of the steady-state gain of $g_1(s)$ is

equal to the sign of $\Theta(0) = 1 - (1 - \gamma_1)(1 - \gamma_2)/\gamma_1\gamma_2$, which changes sign when the process operating condition switches from minimum phase to non-minimum phase and vice versa (that is, when $\gamma_1 + \gamma_2$ crosses 1).

This local instability causes the initial decrease in tank levels. Decreasing the tank levels changes the relative magnitudes of the total flow rates between the top two tanks and the bottom two tanks, causing the right-half-plane transmission zero to move back into the left-half plane, the steady-state gain to change back to its original sign, and the closed-loop poles to move back into the left-half plane. The closed-loop system stabilizes, causing the tank levels to increase back towards the desired setpoints. This switch from closed-loop stability to instability and back to stability is why the initial decreases followed by increases in the tank levels are sharper than expected for a smooth system consisting of only low-order processes. There is no apparent “inverse response” in either control loops when stepping down the setpoint. While hysteresis is common in industrial process units such as valves, the case here is more interesting because it involves the movement of a transmission zero between the left- and right-half planes and a change in sign of the steady-state gains, resulting in very poor closed-loop performance obtained for a linear controller. (Although the essence of the argument is valid, for the student’s sake this interpretation involves some simplification, since the real system is nonlinear.)

For this particular valve knob setting, the full decoupling controller induces this behavior more readily than the decentralized or partial decoupling controller. This illustrates the important point that when interactions are large enough, decoupling control can do more harm than good.^[8,9] Full decoupling control has increased sensitivity to uncertainties in the transfer function model, which causes the ratios of the total flow rates in the bottom tanks and top tanks to vary more than for the other controllers. If the valve knob is shifted so that the transmission zero easily moves between the right- and left-half planes for the whole operating range (instead of only for some conditions, as in Figures 8 and 9), then good setpoint tracking is unobtainable by a linear controller, no matter how sophisticated.^[9]

The second important point is that hysteresis effects are common in industrial control loops and should be considered when troubleshooting. The third point is that the cause of unexpected dynamic behavior in control loops is often more subtle than what is often first assumed. But such phenomena can be understood with some thinking and judicious application of undergraduate-level process control analysis tools. This understanding is needed to determine whether a particular control problem can be resolved by better controller tuning, a different control structure, by changing the process design, or by changing the operating conditions.

For the next experiment, the quadruple-tank process was made more interactive by using the Y-junctions to increase

the proportion of flow to the top tanks. Closed-loop responses with decentralized control are shown in Figure 10. Due to the higher interactions, as well as some nonlinear effects, the closed-loop responses were highly oscillatory around the setpoints. The student was unable to obtain controller tuning parameters that would stabilize the closed-loop system when either steady-state or dynamic decoupling was used. The best closed-loop response obtained by dynamic decoupling is shown in Figure 11. The initial closed-loop performance was acceptable up to 200 s, but the level in Tank 2 deviated from

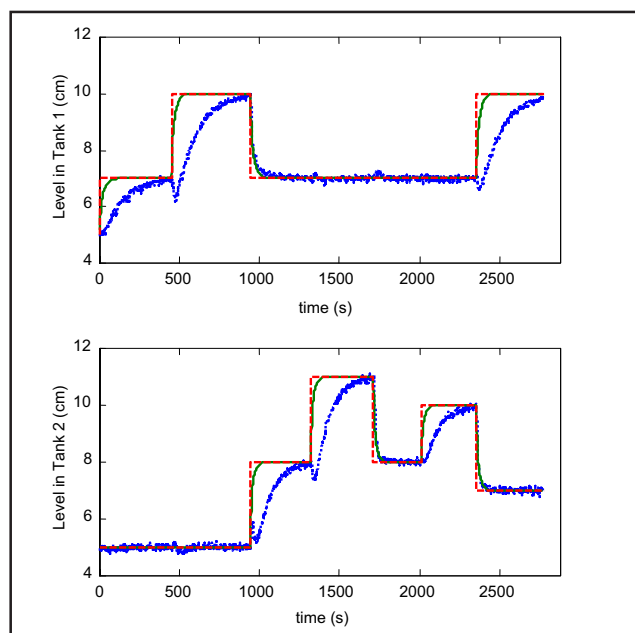


Figure 8. Full decoupling with aggressive tuning: setpoint (dashed line), experiment (dots), model prediction (solid line).

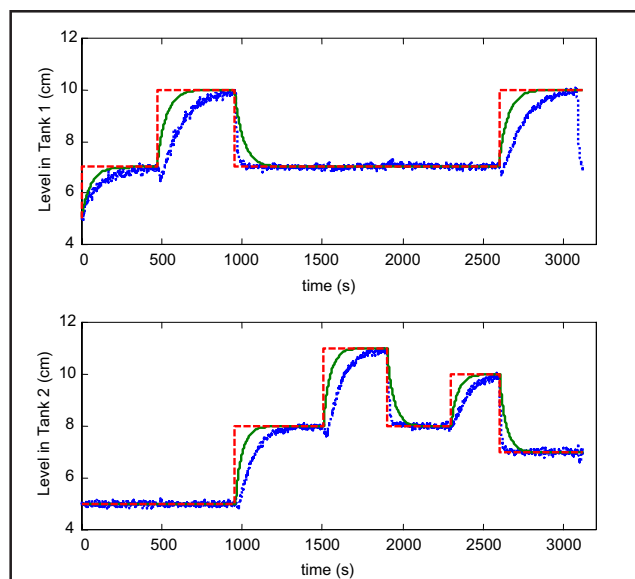


Figure 9. Full decoupling with sluggish tuning: setpoint (dashed line), experiment (dots), model prediction (solid line).

the setpoint for $t > 400$ s, indicating that the closed-loop system was not locally asymptotically stable. In addition, there was a consistent steady-state offset exhibited by the level in Tank 1. Again, this illustrates to students that a process that is designed poorly can be difficult or impossible to control.

Different student teams are given different valve settings in the Y-junctions, and students are encouraged to share their results with other teams. Students who consistently have $>80\%$ of the flow going to the bottom tanks observe that decoupling control can provide better closed-loop performance than multiloop control. Decoupling control performs worse than decentralized control when the interactions are increased. When the total flows to the top and bottom tanks are equal or nearly equal, no linear controller can provide acceptable closed-loop performance.

CONCLUSIONS

A 4-tank apparatus was introduced in which a multivariate transmission zero can cross the imaginary axis during a single closed-loop response, which is used to illustrate the effects of time-varying dynamics, changes in the sign of the steady-state gain, and hysteresis. Example student results illustrated how the apparatus is used to teach many important points that are ignored in most process control lectures and laboratories: 1) the effect of time-varying dynamics should be considered when designing control systems; 2) the sign of the steady-state gain should always be considered when designing control systems for multivariable processes; 3) the cause of unexpected dynamic behavior in control loops is often more subtle than what is first assumed; 4) under some conditions, full decoupling can lead to significantly worse performance than partial decoupling; 5) decoupling control can do more harm than good; 6) hysteresis effects should be considered when troubleshooting control problems. This level of understanding is needed for students to select

the proper multivariable control structure and to determine whether a particular control problem can be addressed by better controller tuning, by a different control structure, by changing the process design, or by changing the operating conditions.

Although not reported here, the apparatus has been used to implement partial and full steady-state decoupling, to compare with dynamic decoupling. Also, it would be educationally valuable to investigate the development of feed-back linearizing controllers to enable a single controller to provide good performance for a wider range of operating conditions.^[15]

ACKNOWLEDGMENT

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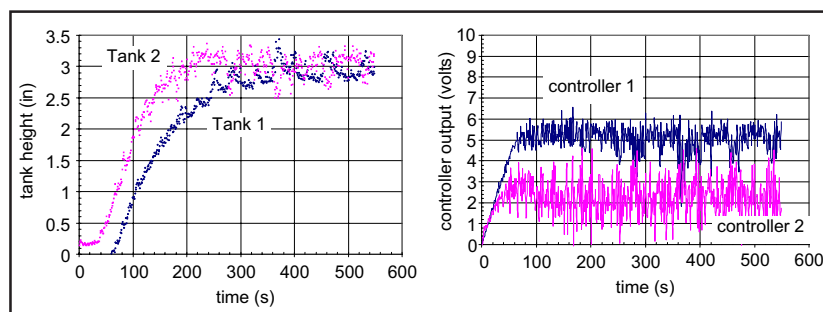


Figure 10. Responses to decentralized control with setpoint heights of 3 inches in a strongly interacting system.

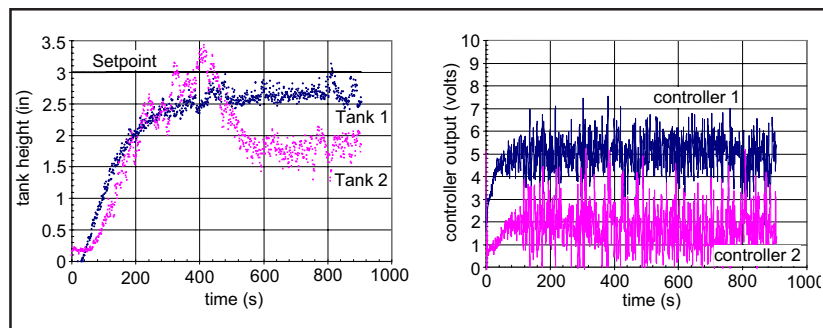


Figure 11. Responses to dynamic decoupling control with setpoint heights of 3 inches in a strongly interacting system.

Simulation and Experiment in

AN INTRODUCTORY PROCESS CONTROL LABORATORY EXPERIENCE

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There are several advantages to integrating classroom and laboratory exposure. For many students, understanding concepts taught in the classroom improves significantly when they have the opportunity to gain hands-on experience in a laboratory. A laboratory exercise also provides an opportunity to apply the theory they have learned in the classroom to an actual engineering problem. Finally, comparing experimental data and dynamic simulation results is an effective way to reinforce process dynamics education in a laboratory exercise. The wider incorporation of process dynamics into the curriculum is considered to be a key component in process control education of chemical engineering students.^[1]

There are a number of simulation-based chemical process dynamics experiments presented in the engineering education literature. They range from modules incorporated into a commercial process control computer system,^[2] case studies illustrating various process control concepts programmed using MATLAB/SIMULINK,^[3-5] and workshops based on real-time simulation of industrial unit operations.^[6] Although there are benefits of simulation-based experiments, a major disadvantage is the lack of an actual physical process that the students can watch, hear, and touch while it is operating. Understanding the dynamic behavior of a process is greatly enhanced by observing the physical process operation. Visualization provides a significant benefit to many students as they attempt to apply the theoretical concepts taught in the classroom.^[7,8] This aspect was one of the main motivations for developing the experience documented in this work.

A review of the equipment-based chemical process dynamics experiments presented in the engineering education lit-

erature reveals a wide range of complexity in the processes considered. They range from relatively simple liquid-level^[9] and stirred-tank^[10] systems, multiple tank systems,^[11] quite complex reaction^[12] and distillation^[13] systems, and combinations of simple, more complex, and simulated systems.^[14] Because this experience is intended to be an introductory exposure to process dynamics, simulation, and control, using an easily modeled, simple, physical process that incorporates the introductory concepts from the process control and simulation course is appropriate. For this reason, a single-tank liquid-level system was chosen.

Feedback control is performed using a proportional-only controller. Proportional control provides two benefits for this introductory experience. The first is that a proportional controller is easily simulated. The additional complexity required in the simulation of integral action in the controller provides little, if any, benefit to the understanding of process dynamics and dynamic simulation in an introductory experience. The second benefit is that proportional control results in steady-state offset of the tank level. This concept is often difficult for some students to initially grasp in the classroom. The ability to observe this phenomenon on a real physical system can be very helpful for these students.

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For many students, understanding concepts taught in the classroom improves significantly when they have the opportunity to gain hands-on experience in a laboratory. A laboratory exercise also provides an opportunity to apply the theory they have learned in the classroom to an actual engineering problem.

LABORATORY EQUIPMENT

The experiment is carried out using a 50-gallon gravity-drained tank equipped with liquid level and outlet flow sensors. Liquid level is controlled by a valve on the inlet water pipe. There is an additional inlet water pipe with a manual valve. The outlet flow rate can be adjusted by a manual valve on the outlet pipe of the tank. A steam heater is connected to the tank but not used in this experiment. The tank is 2.5 feet in height and 1.8 feet in diameter. The tank system is shown in Figure 1.

Liquid level control is provided by a single-loop electronic controller. There is also a distributed computer control system connected to the tank. Because we believe there is value in exposing the students to both the single-loop electronic and computer control systems, we have the ability to switch between the two systems on this tank. The single-loop controller is used for this introductory experiment, while the computer control system is used for temperature-control experiments and a model predictive control experiment in the senior laboratory course.^[15]

LABORATORY EXERCISE

The exercise comprises two three-hour laboratory sessions. During the first session, the student groups become familiar with the tank system and perform the experimental work. In the second session, they develop their dynamic simulation model, compare their simulated results with those obtained experimentally, and document their findings in a short memo report to the instructor.

The laboratory exercise begins with the tank operating at steady state under proportional-only feedback control with a water level setpoint of 50%. The instructor reviews the physical operation of the tank, goes over each component comprising the feedback control loop, and leads a short discussion concerning the options to remove steady-state offset with the student group. The students are then instructed to adjust

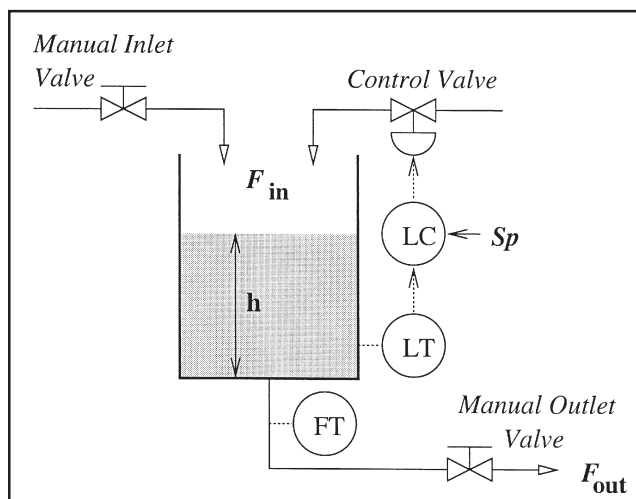


Figure 1. Experimental tank system.

the controller bias to remove the steady-state offset in the tank level. They may either put the controller in manual and adjust the control valve position or adjust the bias directly to eliminate the offset. The value of this exercise is gaining an appreciation for the response time of a real physical system. The students are prompted to estimate both the time constant of the system, which is on the order of five minutes, and the open-loop response time of the tank in order to determine how long it should take for the tank level to reach steady state after a

change to the inlet water valve position is made. Although process simulators provide valuable training experience for the students, a major drawback is that those experiences are in “simulation” time. The first part of this laboratory exercise demonstrates that real process dynamics are not on this same simulation time scale.

After the students have adjusted the bias to eliminate the steady-state offset in the tank level, the system is returned to closed-loop control and they are allowed to choose one disturbance from a list in the laboratory instructions. This list contains the following disturbances:

- Simultaneously dump two small buckets of water into the tank
- Dump one large bucket of water into the tank
- Change the inlet flow rate by opening the manual disturbance flow valve
- Change the outlet flow rate by opening or closing the manual outlet valve
- Change the level setpoint
- Change one of the level controller tuning parameters

where the two small buckets are each two gallons, resulting in an impulse disturbance that is approximately 20% of the liquid volume; the large bucket is 25 gallons, resulting in an impulse disturbance when full that is about the same as the liquid volume; and the disturbance flow results in a step

disturbance that is about the same as the initial steady-state inlet flow rate.

From the instructor's perspective, it is desirable to have as much variation in the selected disturbances between groups as possible to make the students' semester-end oral reports on this experiment more interesting. In practice, other than discouraging the one large bucket, prompting by the instructor in order to provide this variation has seldom been necessary.

Prior to implementing their chosen disturbance, the tasks of time keeper, data logger, and disturbance initiator are distributed by the group members among themselves. Their selected disturbance is then implemented on the tank system under closed-loop level control. The initial data point is collected after the disturbance has been completed. In the case of the buckets, this point is the time when all of the water has been emptied into the tank. Because two students (and sometimes the instructor) are required to empty the bucket contents into the tank, the time-keeping and data-logging tasks are performed by one student at the beginning of the experiment. For the other disturbances, the initial data point is taken immediately after the valve position or controller tuning parameter has been changed. Data is collected at intervals of ten to twenty seconds until the tank level reaches steady state. The experimental phase of this exercise is typically completed well within the three-hour laboratory period.

PROCESS SIMULATION

The second phase of this exercise involves the dynamic simulation of the closed-loop tank system with the disturbance chosen by the group. This phase is carried out during the laboratory period immediately following the experimental session. Process simulation begins with an unsteady-state material balance over the tank. Assuming a constant cross-sectional area of the tank, A_c , and the same constant density for all water streams, a macroscopic mass balance results in

$$A_c \frac{dh}{dt} = F_{in} - F_{out} \quad (1)$$

where h is the height of water in the tank, F_{in} is the inlet volumetric flow rate, and F_{out} is the outlet volumetric flow rate.

The inlet volumetric flow rate of water is determined by the position of the control valve. Although this control valve is linear, the inlet flow rate is not a linear function of valve position over the entire valve position range due to variation in the water supply pressure as the valve position changes. The students are given a calibration curve, shown in Figure 2, that is used to relate the inlet flow rate to the control valve position. Over the linear operating range of the valve, the following correlation can be used to deter-

mine the inlet flow rate

$$F_{in} = 0.171(V_p) - 1.03 \quad 10 \leq V_p \leq 60 \quad (2)$$

where F_{in} is the flow rate in units of gpm and V_p is the control valve position in units of % open. If the disturbance flow was selected, there is a second constant inlet flow rate that must be added to this relationship.

The outlet volumetric flow rate is assumed to be proportional to the square root of the pressure drop across the manual outlet valve due to the static head of fluid in the tank

$$F_{out} = K_v \sqrt{h + \frac{19}{12}} \quad (3)$$

where F_{out} is the flow rate in units of gpm, K_v is the proportionality constant, h is the height of the water in the tank in units of feet, and the bottom of the tank is 19 inches above the outlet valve. The proportionality constant K_v is determined from the measured outlet flow rate and water height when the tank level is at steady state.

The control valve position is determined by the level controller on the tank. For the proportional-only controller, the valve position is determined from the controller equation

$$V_p = B + K_c(S_p - L) \quad (4)$$

where V_p is the valve position in units of % open, B is the controller bias in units of % open, K_c is the proportional gain in units of % open/% level, S_p is the water level setpoint in units of % level, and L is the level of the water in the tank in units of % level. In practice, the controller gain is kept at a value around 1 %/% to prevent the control valve position from moving out of its linear operating range during the transient response due to the disturbance.

Simulation of the process is carried out by numerical solution of Eqs. (1) through (4). Before they can be solved, however, the units must be made consistent throughout all of the

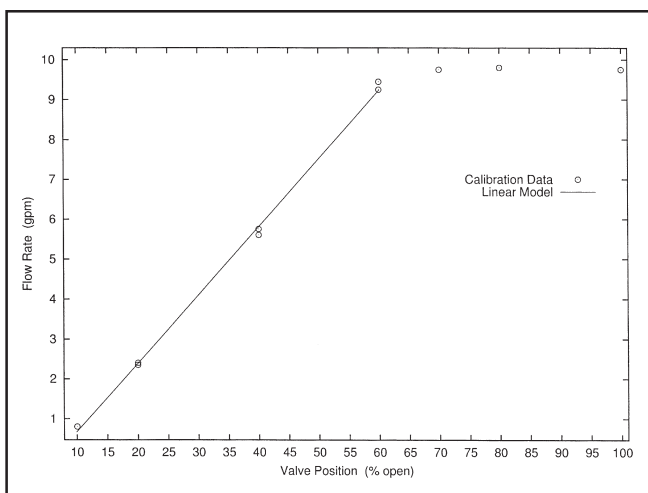


Figure 2. Inlet water control valve calibration curve.

relationships. The controlled variable for the controller is configured to be in units of % while the tank dimensions are given to the students in units of feet and the flow rate calibrations are given in units of gpm. This variation in the units given to the students is intentional. Numerical solution is typically carried out by the student groups using MathCad, which is used by the department in the introductory material balance and the numerical methods prerequisite courses, although they are free to use any of the other mathematical software packages such as MATLAB, EXCEL, and Maple that are available on the engineering college server.

EXAMPLES AND DISCUSSION OF RESULTS

Example experimental and simulation results are shown in Figures 3 and 4. Figure 3 presents the results for the large bucket impulse disturbance. In this example, the large bucket was only about half full. Figure 4 presents the results for a reduction in the outlet flow rate from closing the manual outlet valve. In

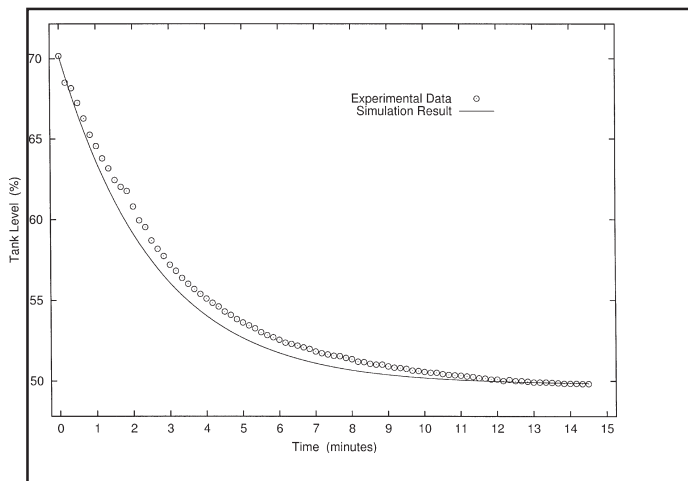


Figure 3. Experimental and simulated closed-loop tank level for the large bucket impulse disturbance.

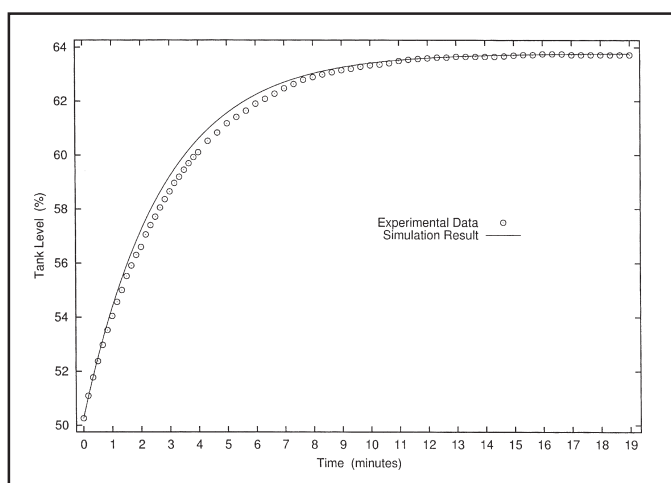


Figure 4. Experimental and simulated closed-loop tank level for a change in the outlet valve position.

both cases, the experimental and simulated responses are very similar. These results are typical for most of the student lab groups.

In addition to presenting their experimental and simulation results, the student groups are asked to discuss the sources of error in this experiment in their group memo report. Examination of the experimental and simulated dynamic responses reveals that the simulation leads the experimental response. Because there are dynamics associated with the level sensor and control valve that are not included in the simulation model, this result would not be unexpected. The effects of valve friction, sensor noise, and the precision of the liquid level value displayed by the controller can also contribute to error as well as the assumption of a perfect square root relationship and a constant K_v value for the outlet flow rate that may not be valid over the liquid level ranges encountered in the experiments. Experimental error in the timing of the collected level data samples is also present. Almost every student group mentions the valve, sensor noise, and sampling error as sources of error in their report. Some groups also mention the outlet flow relationship used in the simulation model. Few groups discuss the dynamic effect of the valve and sensor.

STUDENT RESPONSE

As part of the student evaluation of the process simulation and control course, a number of supplemental questions concerning the value of the text and controller simulation software used in the course, the laboratory experience documented here, and the preparation received in the required prerequisite courses are included. The evaluation scores ranged from 5=Very Effective to 1=Very Ineffective. The average scores from the last four years are: presentation and explanation of concepts in the textbook, 3.04; use of CStation for class examples, 3.25; use of CStation for homework problems, 2.96; process control experiment in Lab II, 4.02.

CStation^[16] is the process control simulation software package used in the course, *Essentials of Process Control*^[17] was the course text at the time of these evaluations, and the process control experiment in Lab II is the experience documented in this work.

The average score given by the students for this laboratory experience is considerably higher than for the text and process control simulation package and is essentially the same as the average score of 4.10 for the value of the process control and simulation course over the same period. It should be noted that a number of students have provided somewhat negative comments concerning the length of the loop tuning homework assignments requiring the use of CStation. These feelings may have had some influence on the CStation scores. It should also be noted that only one

Continued on page 315.

valuable in industry and could be useful in academe (e.g., which centers should the university compete for?). Asking questions is valuable—how long do professors need for different tasks, what can be done to improve the process, if students aren't the customers, who is, etc. Industrial faculty members can help ask the questions and help search for answers.

SUMMARY

Many chemical engineering departments have been criticized for a lack of industrial experience in their faculty. One

approach to partially solving this problem is to hire early retirees from industry. As shown by the experiences related in this paper, these returning professors will probably experience some degree of cultural shock. Their transition to becoming productive contributors can be eased by providing both formal training in teaching and informal mentoring.

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Process Control Laboratory Experience

Continued from page 309.

student provided written comments about the text and that no student provided written comments about the laboratory experience over the four-year period. Because there are no formal course evaluations for laboratory courses, student response data from the second-semester junior laboratory course concerning the laboratory course and this experiment is not available. Qualitative assessment of this experience based on comments received from the students during and after the experiment indicate that this experience has been generally well received by the students.

CONCLUSIONS

An introductory laboratory experience in process dynamics and control that is conducted concurrently with the process simulation and control course at Villanova University has been presented here. The experience is intended to reinforce the introductory concepts of dynamic simulation and feedback control presented in the classroom by using a simple liquid-level process. Based on quantitative and qualitative student responses in the laboratory and process simulation and control courses, the students found the experience a valuable addition to their process simulation and control education.

ACKNOWLEDGMENTS

A curriculum revision grant to the Villanova University Chemical Engineering Department from Air Products and Chemical Co. that supported development of this laboratory experience, and the contributions of Professor Robert Sweeney in the design and construction of the experimental system are gratefully acknowledged. I would also like to thank the Villanova University chemical engineering students over the past four years for their active participation in the continuing development and improvement of this experience, and Ami Badami and Jenny Papatolis of the class of 2003 for supplying their respective group's experimental and simulation results that are presented in this paper.

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USE OF DYNAMIC SIMULATION TO CONVERGE COMPLEX PROCESS FLOWSHEETS

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Commercial process simulators are widely used for designing new processes and for analysis of existing processes. Most senior design courses contain a significant component of computer simulation of process flowsheets using these tools. The most widely used commercial process simulation software is that developed by Aspen Technology—AspenPlus for steady-state simulation and AspenDynamics for dynamic simulation—and these tools are used in the examples in this paper. The standard Aspen notation is used. For example, distillation column stages are counted from the top of the column: the condenser is Stage 1 and the reboiler is the last stage.

The simulators contain models of most common unit operations, which can be connected into a process flowsheet. If the units operate in series, with upstream units feeding downstream units, the simulation is usually reasonably straightforward. If the flowsheet contains recycle streams, however, the simultaneous solution of the typically very large number of simultaneous nonlinear algebraic equations that make up the steady-state model can be quite challenging. There is no guarantee that any algorithm will find a solution. In addition, there are sometimes multiple solutions in these nonlinear systems. The convergence of these recycle loops (or “tear” streams) is a major challenge in steady-state process simulation.

Energy integration can also produce complications because of “energy recycle” between different units. These difficulties can sometimes be avoided by using the plant utility system to break the energy linkage.

Commercial steady-state simulators contain a variety of algorithms. For example, the user of AspenPlus can try such methods as Wegstein, Broyden, and Newton. Convergence tolerances and the maximum number of iterations can also be adjusted.

The experience of many users, particularly students, has been that the convergence of recycle loops is the most diffi-

cult part of steady-state simulation. The normal procedure is to assume some conditions of a recycle stream (flow, temperature, pressure, and composition) and work down through the flowsheet until the calculated values of the recycle stream are available. If the assumed and calculated values are not sufficiently close, new guesses must somehow be made. The process is repeated until convergence between the assumed and calculated values has been attained. Often, however, convergence does not occur.

One would think that this convergence should be fairly easily achieved if the user has adjusted the design and operating parameters so the assumed and calculated conditions of the recycle stream are fairly close, but this all too frequently does not occur. For example, in one of the cases discussed later, an assumed recycle stream had a composition 98 mol% methanol and 2 mol% water, while the calculated stream is only slightly different (0.4 mol% dimethyl ether; 97.2 mol% methanol; 2.4 mol% water). The assumed flowrate is 72 kmol/hr, while the calculated flowrate is 72.9 kmol/hr. The temperature and pressures are identical. After connecting the recycle stream and defining it as a “tear” stream in the “Convergence” section of the “Data Browser” in AspenPlus, the recycle loop does not converge when using any of the algorithms.

This paper illustrates that recycle loops can be easily converged if the steady-state AspenPlus simulation (with the re-



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cycle loops not connected) is “exported” into the dynamic simulator AspenDynamics and the recycle connections are made on the dynamic model. The steps in going from a steady-state simulation to a dynamic simulation are discussed in the next section.

It should be noted that the issue of requiring good initial guesses of plant conditions in order to converge is not a problem since all the units have been converged individually in AspenPlus before going into dynamics. The “guessed” and the “calculated” values of the tear streams have also been adjusted to be fairly close to each other.

TRANSITION FROM STEADY STATE TO DYNAMIC SIMULATION

There are several items that must be taken care of to convert a steady-state simulation into a dynamic simulation: all equipment must be sized and a control structure must be developed. Luyben^[1] presents many details of these necessary steps, which are summarized below. Not all of the units that are available in steady-state AspenPlus are supported in AspenDynamics, so this limitation must be kept in mind. For example, neither the “separator” (a fictitious component splitter) nor a liquid-liquid extractor is supported in the current version (Version 11.1) of AspenDynamics.

When the steady-state simulation in AspenPlus is exported into AspenDynamics, a “pressure-driven” dynamic simulation should be used. This requires that all the “plumbing” must be specified in the flowsheet. Pumps and compressors must be inserted where needed to provide the required pressure drop for material flow. Control valves must be installed where needed, and their pressure drops selected.

This is one of the more important educational aspects of the procedure since most students have a poor grasp of plumbing. Common errors include inserting two valves into a liquid-filled line, inserting a valve in the suction of pumps, or inserting a valve at the discharge of compressors (compressor speed or its equivalent compressor work should be manipulated).

Equipment Sizing • For steady-state simulation, the size of the equipment is not needed, except for reactors. For dynamic simulation, the inventories of material contained in all the pieces of equipment affect the dynamic response, so the physical dimensions of all units must be known.

In distillation columns, the diameter of the column, the weir height, and the sizes of the reflux drum and the column base must be specified. Of course, before these can be calculated, the number of stages and the feed stage location must be set by some heuristic or rigorous optimization method. Perhaps

the easiest heuristic approach is to fix the distillate and bottoms specifications (using the *Design Spec* and *Vary* tools in AspenPlus) and keep increasing the number of stages until the required reflux ratio stops decreasing—this gives the minimum reflux ratio. Then the actual reflux ratio is set at 1.2 times this minimum. Finally, the optimum feed stage can be determined by varying the feed stage until the minimum reboiler energy consumption is found.

The *Tray Sizing* section of a distillation column block in AspenPlus can be easily used to provide the column diameter. The default weir height of 0.05 m can be used. The volumetric flowrates of liquid into the reflux drum (Stage 1, the “condenser” in Aspen terminology) and the liquid into the base of the column (the last stage, or “sump” in Aspen terminology) can be used to size the two vessels by using the heuristic of a 10-minute holdup time. These volumetric flowrates are given in the *Hydraulics* page tab of the *Profiles* section of the column block. To have these results made available, you must go to the *Report* section of the column block, select the *Property Options* page tab and click the *Include Hydraulic Parameters* box before running the program.

For example, the liquid holdup in the reflux drum of a column with a total condenser is calculated from the volumetric flowrate of liquid leaving the drum (distillate plus reflux).

$$[\text{Drum volume (m}^3\text{)}]$$

$$= [\text{Liquid volumetric flowrate (m}^3/\text{min)}][10 \text{ minutes}]$$

If an aspect ratio (length to diameter, L/D) of 2 is used, the diameter of the drum is

$$D = [2(\text{Volume})/\pi]^{1/3}$$

The same procedure can be used for flash tanks and vaporizers. Flash tank vapor velocity should also be checked.^[2]

Heat exchanger tube-and-shell volumes can be calculated from the heat-transfer area, which is known from the steady-state design, if a tube diameter D (typically 0.0245 m) is selected.

$$\text{Area} = [\text{number of tubes}][\pi D][\text{tube length } L] = N_{\text{tube}}(\pi DL)$$

$$\begin{aligned} [\text{Volume of tubes}] &= [\pi D^2/4][L][N_{\text{tube}}] \\ &= [\pi D^2/4][L][\text{Area}/[\pi DL]] = D[\text{Area}]/4 \end{aligned}$$

Shell volume is approximately equal to tube volume in most tube-in-shell heat exchangers. If the process streams in the heat exchanger are gases, the dynamics are very fast and can usually be ignored (specify *Instantaneous* in the Dynamic section of the heat-exchanger block).

Plantwide Control • When the file containing the flowsheet is opened in AspenDynamic, a default control scheme is al-

The convergence of steady-state simulations of flowsheets with recycle streams is frequently very difficult. An alternative is suggested in this paper and an example illustrates the proposed method.

ready installed on some loops. For example, level and pressure controllers are inserted on all distillation columns and reactors in the flowsheet. This default control must be modified and supplemented with other control loops to incorporate a stable basic regulatory control structure.

- **Plantwide Control Structure** A simple heuristic method for development of an effective plantwide control structure is presented by Luyben, *et al.*^[3] General principles and many examples are given in great detail. The proposed nine-step procedure has been successfully applied to a large number of realistically complex industrial processes. Some of the key concepts are: (1) the control structure should guarantee that all chemical components fed into the system are either reacted or can leave in some exiting stream; (2) a flow controller should be installed somewhere in all liquid recycle loops; and (3) all liquid levels must be controlled and pressures in gas systems, which can be multiple units connected together, must be controlled.

- **Controller Tuning** Most of the controllers are easily tuned by simply using heuristics. All liquid levels should use proportional-only controllers with a gain of 2. All flow controllers should use a gain of 0.5 and an integral time of 0.3 minutes (also enable filtering with a filter time of 0.1 minutes).

The default values in AspenDynamics for most pressure controllers seem to work reasonably well. Temperature controllers often need some adjustments. The default transmitter ranges are usually too large, and spans should be set at about 10% of the absolute temperature level (typically a span of 100 K for moderate-temperature processes).

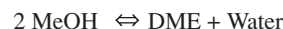
Distillation columns are typically controlled by manipulating reboiler heat input to control the temperature on some selected tray. The heuristic procedure of finding a tray where the temperature changes from tray to tray are large is easy to use and provides effective composition control in most cases. Direct composition measurements can be used if temperature changes are too small. If very large temperature changes occur in the column (over 100 K), an average temperature can be used (measuring the temperatures at three or four trays, calculating the average, and using this for control).

It should be kept in mind that the objective at this point is not to come up with the “best” control structure or the optimum controller tuning. We only need a structure and tunings that drive the simulation to a steady state.

EXAMPLE (“DME” PROCESS)

To illustrate the use of a dynamic simulator to converge a flowsheet, we select the dimethyl ether (DME) process discussed by Turton, *et al.*^[4] This design text gives a flowsheet and some preliminary design param-

eters. The chemistry is the exothermic reversible decomposition of methanol to form DME and water in an adiabatic, tubular, gas-phase reactor.



The reaction is exothermic, and the adiabatic temperature

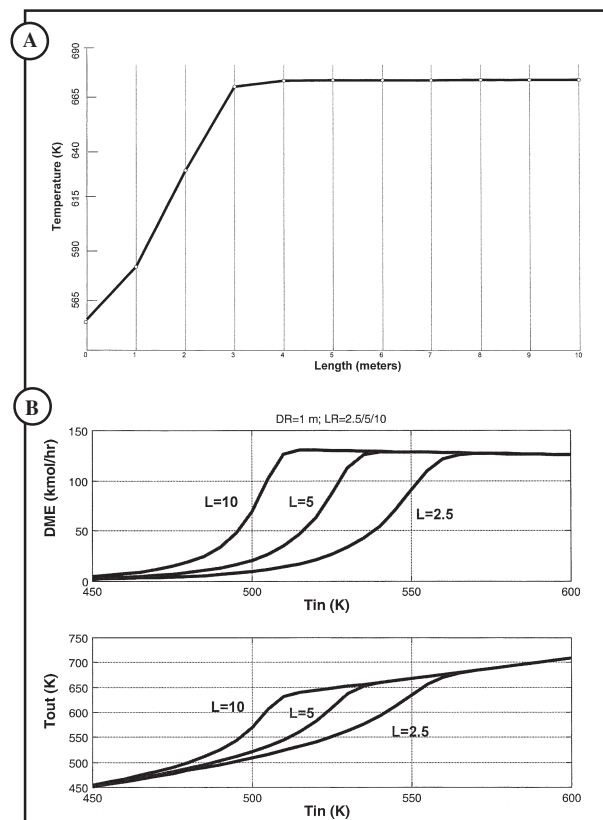


Figure 1.
(A) Adiabatic reactor temperature profile (10 meters length).
(B) Effect of inlet temperature for different reactor lengths.

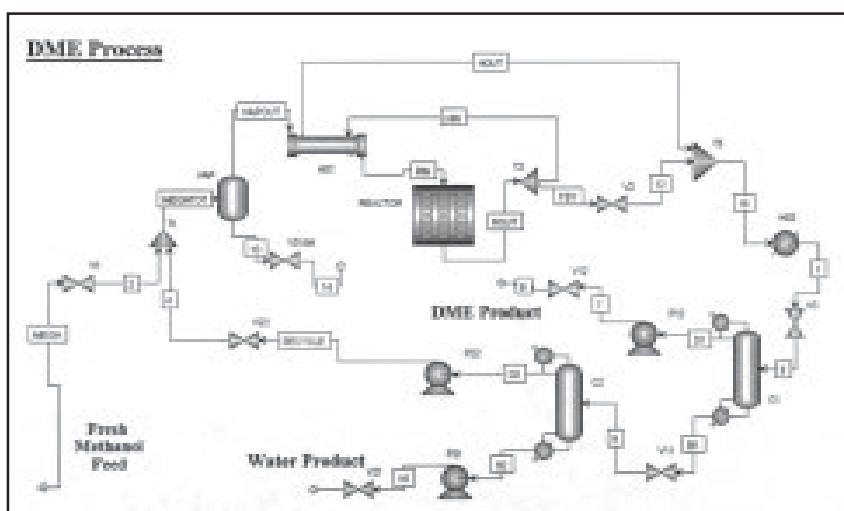


Figure 2. DME flowsheet.

rise is about 120 K. The temperature profile is shown in Figure 1A for a reactor that has a diameter of 0.72 m and is 10 m long. Figure 1B shows how reactor inlet temperature T_{in} affects the production of DME and the reactor exit temperature T_{out} for three different reactor lengths. The inlet temperature required to achieve maximum conversion decreases as the reactor is made bigger. Since the reaction is exothermic, the maximum conversion decreases slowly as temperatures increase.

The equilibrium constant is about 6 at a reactor temperature of about 600 K, so the per-pass conversion is about 80%. This requires a recycle of methanol back to the reactor from the separation section. Figure 2 gives the AspenPlus flowsheet, and Figure 3 gives stream conditions. The NRTL physical property package is used in the simulation.

Fresh methanol and recycle methanol are vaporized and heated to 555 K. The vapor-phase reaction occurs at about 15 atm. Reactor effluent is cooled and fed into a two-column separation section. The low-boiling DME is the distillate product in the first column C1, which operates at a pressure of 10 atm so that cooling water can be used in the condenser (reflux-drum temperature is 318 K with 99.9 mol% DME purity). The column has 32 stages, is fed on Stage 15, and is operated with a reflux ratio of 0.5.

The bottoms of Column C1 is fed to the second column C2 in which water is removed from the bottom and recycled methanol is removed from the top. This column operates at 1.1 atm and has a reflux-drum temperature of 340 K. It has 22 stages and a reflux ratio of 1.5.

Reaction Kinetics • One of the most difficult parts of developing a flowsheet is getting the reaction kinetic parameters correctly specified. Any errors in unit conversions are

amplified by the exponential expressions.

Since the reaction is reversible, both the forward and the reverse reaction rates must be specified. Thurton, *et al.*,^[2] provide a kinetic expression for the forward reaction rate

$$R_F (\text{kmol} / \text{hr} / \text{m}^3) = 1.21 \times 10^6 e^{-80,480/RT} P_{\text{MEOH}} \quad (1)$$

where P_{MEOH} has units of kPa and the activation energy has units of kJ/kmol. Aspen insists on expressing reaction rates in kmol/sec/m³, so we must divide by 3600. More seriously, Aspen also insists that partial pressure be in Pa, not in kPa. A common error is to multiply by 1000 to convert the pressure in Eq. (1) from kPa to Pa. This is incorrect. The pressure in Eq. (1) is in kPa, and Aspen uses Pa, so the pre-exponential factor must be divided by 1000.

$$\begin{aligned} R_F (\text{kmol} / \text{sec} / \text{m}^3) &= 1.21 \times 10^6 e^{-80,480/RT} [P^{\text{kPa}}] / 3600 \\ &= 1.21 \times 10^6 e^{-80,480/RT} \left[\frac{P^{\text{Pa}}}{1000} \right] / 3600 \\ &= 0.3361 e^{-80,480/RT} P^{\text{Pa}} \end{aligned} \quad (2)$$

Turton, *et al.*,^[4] also give information about the equilibrium constant, but state that the published data does not seem to match the calculations using free energies. This was confirmed by running an *R-Gibbs* reactor in AspenPlus, which gave a much lower reactor conversion than would be predicted by the published data.

The heat of reaction is $\lambda = -11,770$ kJ/kmol, so we can estimate the activation energy of the reverse reaction from that of the forward reaction.

$$E_F - E_R = \lambda \Rightarrow E_R = 80,480 - (-11,770) = 92,250 \text{ kJ/kmol} \quad (3)$$

	MEOH	RECIRC	PN	POUT	DI	DI	DI	DI	DI
Substream Molar									
Substream Flowrate									
DI-MT-1	1.0	5.547E-4	5.547E-4	1.000E-1	1.000E-1	5.547E-4	5.547E-4	5.547E-4	1.000E-1
MEOH	252.000	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1
DI-MT-2	1.0	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1
Substream Flowrate									
DI-MT-1	1.0	7.152E-1	7.152E-1	3.000E-1	3.000E-1	7.152E-1	7.152E-1	7.152E-1	3.000E-1
MEOH	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1
DI-MT-2	1.0	6.610E-1	6.610E-1	3.000E-1	3.000E-1	6.610E-1	6.610E-1	6.610E-1	3.000E-1
Total Flowrate	252.000	1.000E-1	1.000E-1	3.000E-1	3.000E-1	1.000E-1	1.000E-1	1.000E-1	3.000E-1
Total Flowrate	252.000	1.000E-1	1.000E-1	3.000E-1	3.000E-1	1.000E-1	1.000E-1	1.000E-1	3.000E-1
Total Flowrate	252.000	1.000E-1	1.000E-1	3.000E-1	3.000E-1	1.000E-1	1.000E-1	1.000E-1	3.000E-1
Temperature	250.000	3.000E-1	3.000E-1	3.000E-1	3.000E-1	3.000E-1	3.000E-1	3.000E-1	3.000E-1
Pressure	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1	1.000E-1
Phase	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Substream	1.000E-1	1.000E-1	1.0	1.0	1.000E-1	1.000E-1	1.000E-1	1.0	1.000E-1

Figure 3. DME stream data.

To find a reasonable pre-exponential factor for the reverse reaction, the conversion data (reactor size; inlet flowrate, temperature, and composition; and exit composition) given Turton, *et al.*, were used to back-calculate this parameter by trial and error. The resulting kinetic expression is

$$R_R \text{ (kmol / sec / m}^3\text{)} \\ = 2.7 \times 10^{-6} e^{-92,250/RT} (P_{\text{DME}})(P_{\text{Water}}) \quad (4)$$

where P_{DME} and P_{Water} have units of Pa.

Thermal Recycle Loop • A feed-effluent heat exchanger (HX1) is used to preheat reactor feed, using a portion (201 kmol/hr) of the hot reactor effluent to heat the vapor from the vaporizer from 427 K to 555 K. Some of the reactor effluent (134 kmol/hr) is bypassed through valve V2 to control reactor inlet temperature.

Thus there is a thermal recycle loop in the process. Unless the reactor effluent stream is known, the HX1 equations cannot be solved. The conventional procedure to get started is to use a tear stream (see Figure 4). We specify a stream “HIN” and provide estimates of its flow (193 kmol/hr), temperature (672 K), pressure (14.4 atm), and composition (40 mol% DME, 20 mol% methanol, and 40 mol% water).

When this flowsheet is converged, the source of “HIN” is changed to the splitter T2 (deleting stream “5” in Figure 4). In the *Convergence* section of the *Data Browser*, we select *Tear* and specify *HIN* to be a tear stream. Then we rerun the program to get the converged flowsheet around the reactor and heat exchanger HX1.

Material Recycle Loop • Figure 5 shows the flowsheet with a tear stream *RECYCLE*, whose stream conditions have been estimated to be 72 kmol/hr, 345 K, 17 atm, 99 mol% methanol, and 1 mol% water. The calculated conditions for stream *RCALC* are only slightly different from those assumed for *RECYCLE* (73.2 kmol/hr, 342 K, 17 atm, 99.3 mol% methanol, and 0.1 mol% water).

The default convergence method

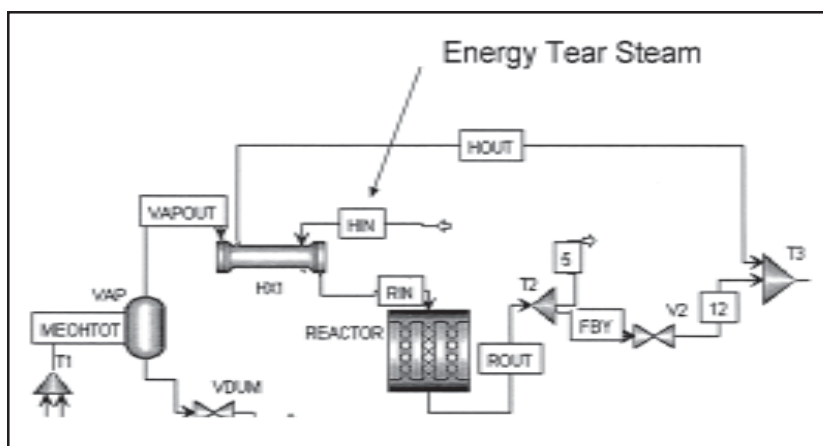


Figure 4. Flowsheet with energy tear stream.

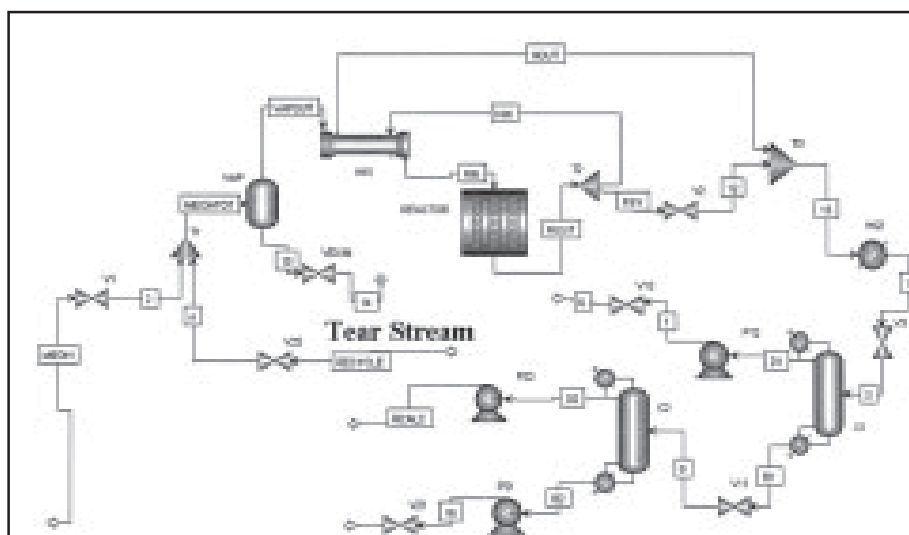


Figure 5. Flowsheet with material tear stream *RECYCLE*.

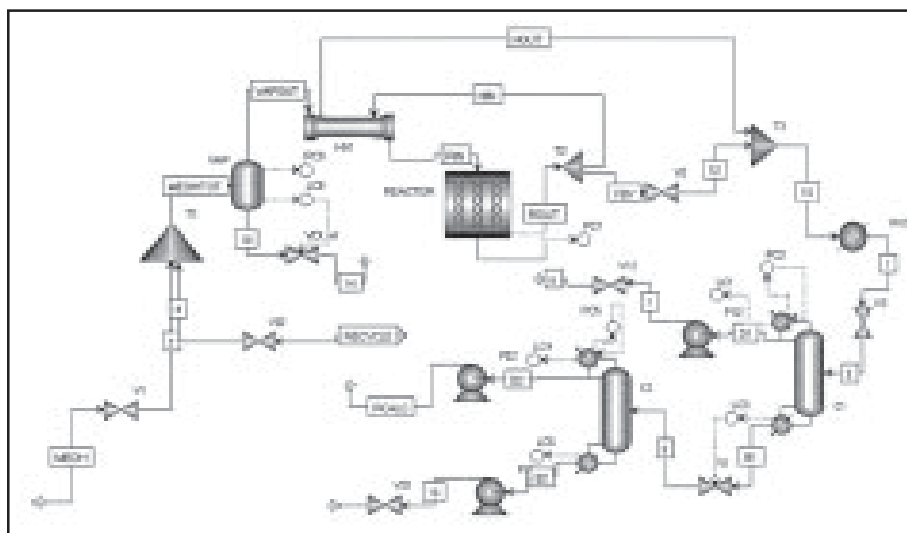


Figure 6. Default control scheme; DME process.

Wegstein is used (with a limit of 30 iterations), the source of the *RECYCLE* stream is specified to be the discharge of pump P22 and it is specified as a *Tear* under the *Convergence Section* of the *Data Browser*. The program is run.

The convergence loop fails to converge.

This is a typical result in many cases. It should be noted that *Design Specs* and *Vary* features are used on both distillation columns. In Column C1, the distillate DME product purity is specified to be 99.9 mol% DME, and the distillate flowrate is varied. In Column C2, the bottoms water product purity is specified to be 99.9 mol% water, and the bottoms flowrate is varied. The reflux ratio is fixed in both columns.

Increasing the maximum iterations does not achieve convergence. Switching to the Broyden algorithm is equally unsuccessful.

This failure to converge certainly does not occur in all cases for all flowsheets, but it does occur in many cases. Senior students spend many frustrating hours trying to get recycle loops to converge.

Converting to Dynamic Simulation • The diameters of the two columns are calculated in the *Tray Sizing* section: 0.61 m for C1 and 0.94 m for C2. The liquid flowrates into the reflux drums of C1 and C2 are 0.242 and 0.131 m³/min, respectively, as found in the *Hydraulics* page tab. Reflux drum sizes (D x L) in the two columns are set at 1.2 x 2.4 m and 1 x 2 m, respectively, using an aspect ratio of 2. The liquid flowrates into the base (to the sump from the next-to-last stage in the column) of C1 and C2 are 0.213 and 0.0853 m³ min, respectively. Reboiler sizes in the two columns are set at 1.1 x 2.2 m and 0.82 x 1.64 m, respectively.

The heat exchangers are assumed to be “instantaneous” since they are gas phase. Reactor size is already specified for the steady-state simulation. The only other dynamic unit in the flowsheet is the vaporizer. Its liquid feed is 10,700 kg/hr with a density of

785 kg/m³, which gives a diameter of 1.1 m and a length of 2.2 m to provide ten minutes of holdup.

The file is pressure checked and exported into AspenDynamics. The default control scheme is shown in Figure 6. Note that each column has pressure and level controllers, some of which are fully connected and others without the controller output signal (OP) connected to a valve. This default control scheme must be modified to provide an effective regulatory control scheme.

Before doing anything, an *Initialization* run and a short *Dynamic* run should be made to confirm that all the plumbing is okay and the process is correctly configured.

Closing the Recycle Loop • The procedure for changing the process structure in AspenDynamics is the same as in AspenPlus. The stream *RECYCLE* is deleted. The destination of the stream *RCALC* is made the inlet to valve V22. Another set of *Initialization* and *Dynamic* runs should be made. Now the default control structure can be modified. It is a good idea to perform *Initialization* and *Dynamic* runs after each new change in the control structure so that any error in controller installation can be detected individually. The most common error is to have the wrong action in the controller (for example, specifying reverse action when it should be direct action).

An obvious alternative to deleting *RECYCLE* and reattaching *RCALC* is to delete *RCALC* and reattach *RECYCLE*. If this is attempted, the little green box at the bottom of the AspenDynamics screen turns red, indicating that something is wrong. Double-clicking the red box opens the window shown at the top of Figure 7, which states that the problem is overspecified. Clicking the *Analyze* button opens the window shown at the bottom of Figure 7, which says that the temperature and pressure of the *RECYCLE* stream must be changed from fixed to variable. Clicking the *ACCEPT* button turns the box green again. Then *Initiation* and *Dynamic* are again run to make sure all is okay. Now the default control scheme can be modified.

Plantwide Control Structure • Using the method proposed in Luyben, *et al.*,^[3] a plantwide control scheme is developed that features the following loops:

- The feed flow to the first column is flow controlled. This puts a flow controller in the liquid recycle loop. It also has the advantage of keeping a fixed steady flow to the column. Since the final DME product is produced in this column, product quality variability is minimized by not permitting disturbances to enter this column.
- The vaporizer level is controlled by manipulating the fresh methanol feed. This guarantees that only the amount of methanol that is being consumed in the reactor will be fed into the process. If more DME production is required, the setpoint of the flow controller on Column C1 feed can be increased. Using reactor inlet temperature to change production is not effective because of the reversibility of the reaction. For example, sometimes increasing reactor inlet

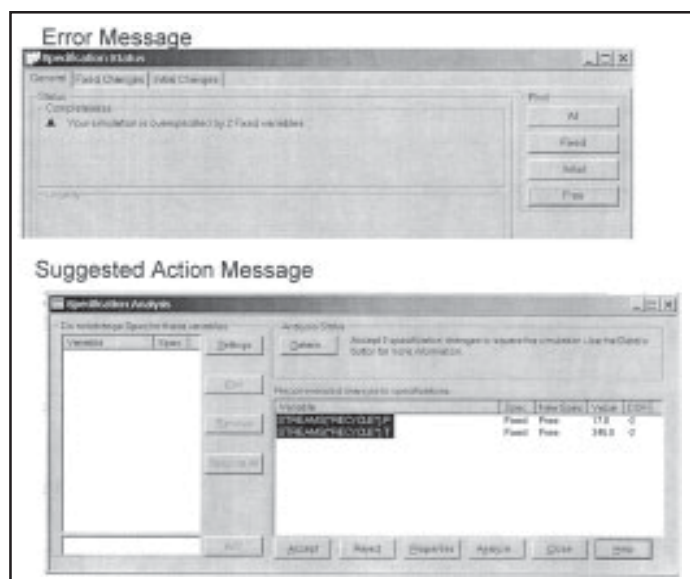


Figure 7. Error message and suggested action message.

temperature produces a decrease in the production of DME.

- Vaporizer pressure is controlled by manipulating steam (heat input Q) to the vaporizer.
- Reactor inlet temperature is controlled by the HX1 heat exchanger bypass flow (valve V2).
- Condenser HX2 exit temperature is controlled by manipulating cooling water (heat removal Q).
- The pressure in each column is controlled by condenser heat removal.
- The reflux-drum level in each column is controlled by manipulating distillate flow.
- The base level in each column is controlled by manipulating bottoms product flow.
- A temperature in each column is controlled by manipulating reboiler heat input. The steep part of the temperature profile in C1 is at Stage 17 and in C2 at Stage 19, so these tray locations are selected. The temperature setpoint in C1 is 380 K and in C2 is 370 K.
- The reflux ratio in each column is controlled. The distillate flowrate is measured, multiplied by the desired reflux ratio (0.5 in C1 and 1.5 in C2) and this signal sets the flowrate of reflux.

Figure 8 gives the

AspenDynamics flowsheet with this control structure installed. All level controllers are proportional with $K_c = 2$. Table 1 gives controller tuning parameters and transmitter spans. The dynamic simulation is run until it reaches a steady-state condition. This may take several “process hours” (several minutes of computer time), depending on the complexity of the flowsheet. When running the dynamic simulation out to a steady state, valve V22 in the recycle line went wide open and the reflux-drum level in Column C2 began to rise. The power to the pump P22 was increased to solve this valve saturation problem. The details of how this is done are given in Luyben.^[1]

The same valve saturation problem occurred in V12 when the

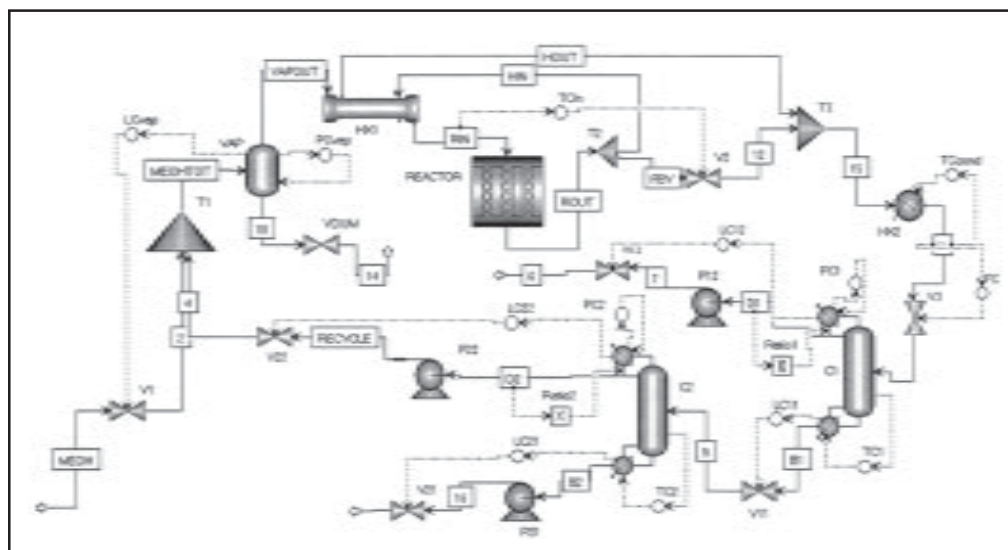


Figure 8. Plantwide control structure: DME process.

TABLE 1
DME Controller Parameters

Controller (Action)	Transmitter Range min/max (units)	Valve Range min/max (Units)	Integral Time τ_i (min)	K_c
FC (Rev)	0/663 (kmol/hr)	0/100 (%)	0.5	0.3
TCin (Dir)	500/600 (K)	0/100 (%)	2	5
LCvap (Rev)	0/3.26 (m)	0/100 (%)	2	
TCcond (Rev)	300/400 (K)	-2030/0 (kcal/sec)	2	20
PCvap (Rev)	10/20 (atm)	0/1910 (kcal/sec)	5	12
TC1 (Rev)	300/400 (K)	0/690 (kcal/sec)	1	20
LC11 (Dir)	0/2.5 (m)	0/100 (%)	2	
LC12 (Dir)	0/3.4 (m)	0/100 (%)	2	
PC1 (Dir)	5/15 (atm)	-442/0 (kcal/sec)	5	12
TC2 (Rev)	300/400 (K)	0/688 (kcal/sec)	1	20
LC21 (Dir)	0/2 (m)	0/100 (%)	2	
LC22 (Dir)	0/2.52 (m)	0/100 (%)	2	
PC2 (Dir)	0/2.2 (atm)	-860/0 (kcal/sec)	20	5

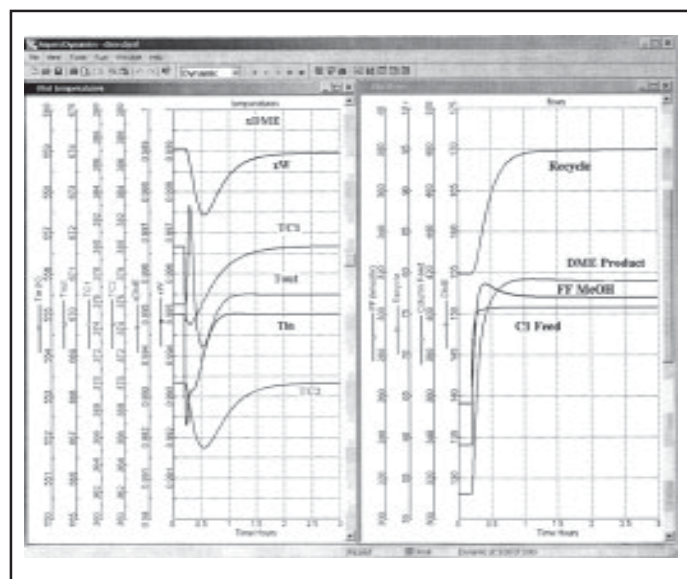


Figure 9. Dynamic responses to 20% increase in feed to column C1.

setpoint of the C1 column feed flow controller was increased 20% (from 236 to 402 kmol/hr). The power to pump P12 was increased. Notice that the steady-state signals to valves V22 and V12 are 20% and 29%, respectively, instead of the normal 50%, because of the higher valve pressure drops.

Figure 9 shows the dynamic response of the system to a 20% increase in column C1 feed. The initial condition is the steady-state condition. The fresh feed of methanol increases from 262 to 308 kmol/hr and DME product increased from 131 to 154 kmol/hr (17.5% increase in production rate). The purities of both the DME and the water products are maintained for this large disturbance. The system takes about two process hours to come to the new steady state.

The one-recycle process illustrates how easily the flowsheet can be converged by using dynamic simulation. Figures 10 and 11 give an example of a process with two recycles. The methyl acetate and butanol reactants not consumed in the reactor are separated in a three-column separation section and recycled in two different streams. More details of this example are available from the author.

CONCLUSION

The convergence of steady-state simulations of flowsheets with

recycle streams is frequently very difficult. An alternative is suggested in this paper and an example illustrates the proposed method. The steady-state simulation is converted into a dynamic simulation, and the recycle loops are converged by letting the dynamic simulation run to steady-state conditions.

The method depends on the development of a base-level regulatory plantwide control structure, which can be obtained by following a simple heuristic design procedure. Simple controller tuning rules can be applied to eliminate detailed and lengthy controller tuning efforts.

There is, of course, an additional benefit for this approach. The dynamic simulation can also be used to look at the dynamic effects of alternative design conditions (flowsheet structure, operating conditions, equipment sizes, etc.). This approach, which is called "simultaneous design," is a design philosophy in which both the steady state and the dynamic performances of a process are considered at all stages of the development of a process. The book by Seider, *et al.*,^[5] discusses this approach in more detail.

NOMENCLATURE

D	diameter
DME	dimethyl ether
E	activation energy
FF	fresh feed
K_c	controller gain
L	length
P_j	partial pressure of component j
TCn	tray temperature controller in column n
T_{in}	reactor inlet temperature
T_{out}	reactor exit temperature
τ_I	integral time constant in PI controller (minutes)
λ	heat of reaction

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2. O'Brien, N.G., and R.G. Franks, "Development and Application of a General Purpose Analog Computer Circuit to Steady-State Multicomponent Distillation," *Chem. Eng.*, **55**, 21 (1958)
3. Luyben, W.L., B.D. Tyreus, and M.L. Luyben, *Plantwide Process Control*, McGraw-Hill (1999)
4. Turton, R., R.C. Baille, W.B. Whiting, and J.A. Shaeiwitz, *Analysis, Synthesis and Design of Chemical Processes*, 2nd ed., Prentice Hall, pg. 939 (2003)
5. Seider, W.D., J.D. Seader, and D.R. Lewin, *Product and Process Design Principles*, John Wiley and Sons, New York, NY(2004) □

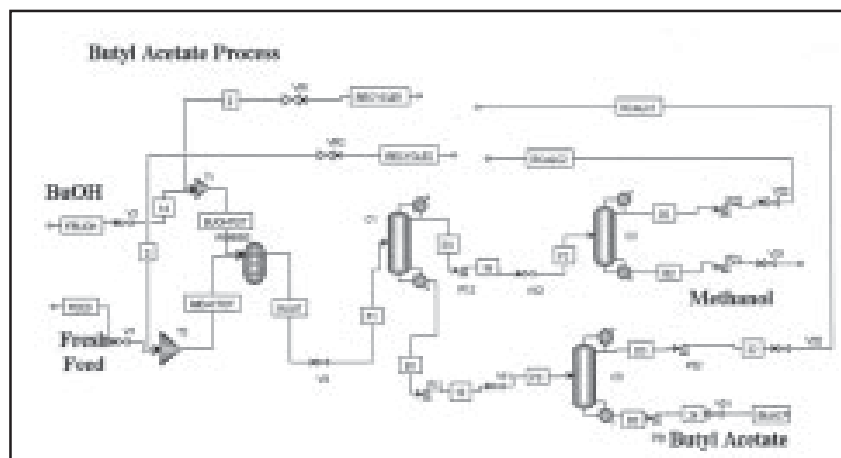


Figure 10. Flowsheet for two-recycle butyl acetate process.

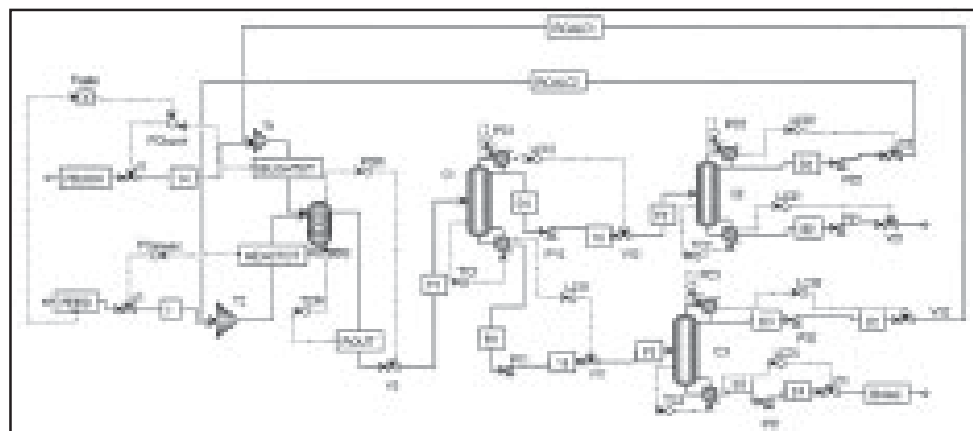


Figure 11. Plantwide control structure for two-recycle process.

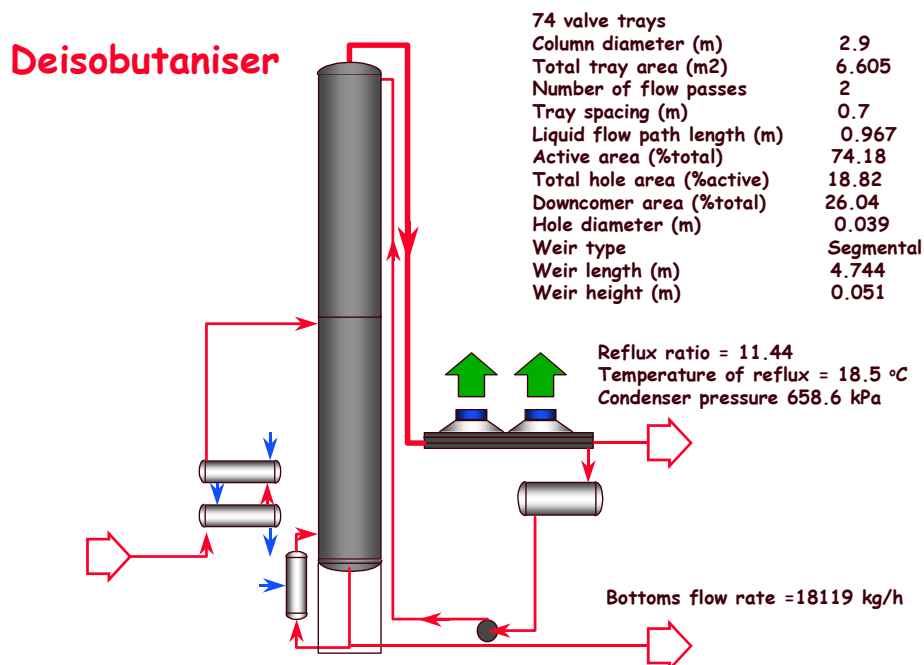
ChemSep 5.0 for Windows!

Harry Kooijman and Ross Taylor

ChemSep is a program for performing multicomponent separation process calculations. *ChemSep* was created specifically for use in courses on thermodynamics and/or separation processes. *ChemSep* integrates flash, the classic equilibrium stage column model and a **nonequilibrium** or **rate-based** column model in one easy to use program.

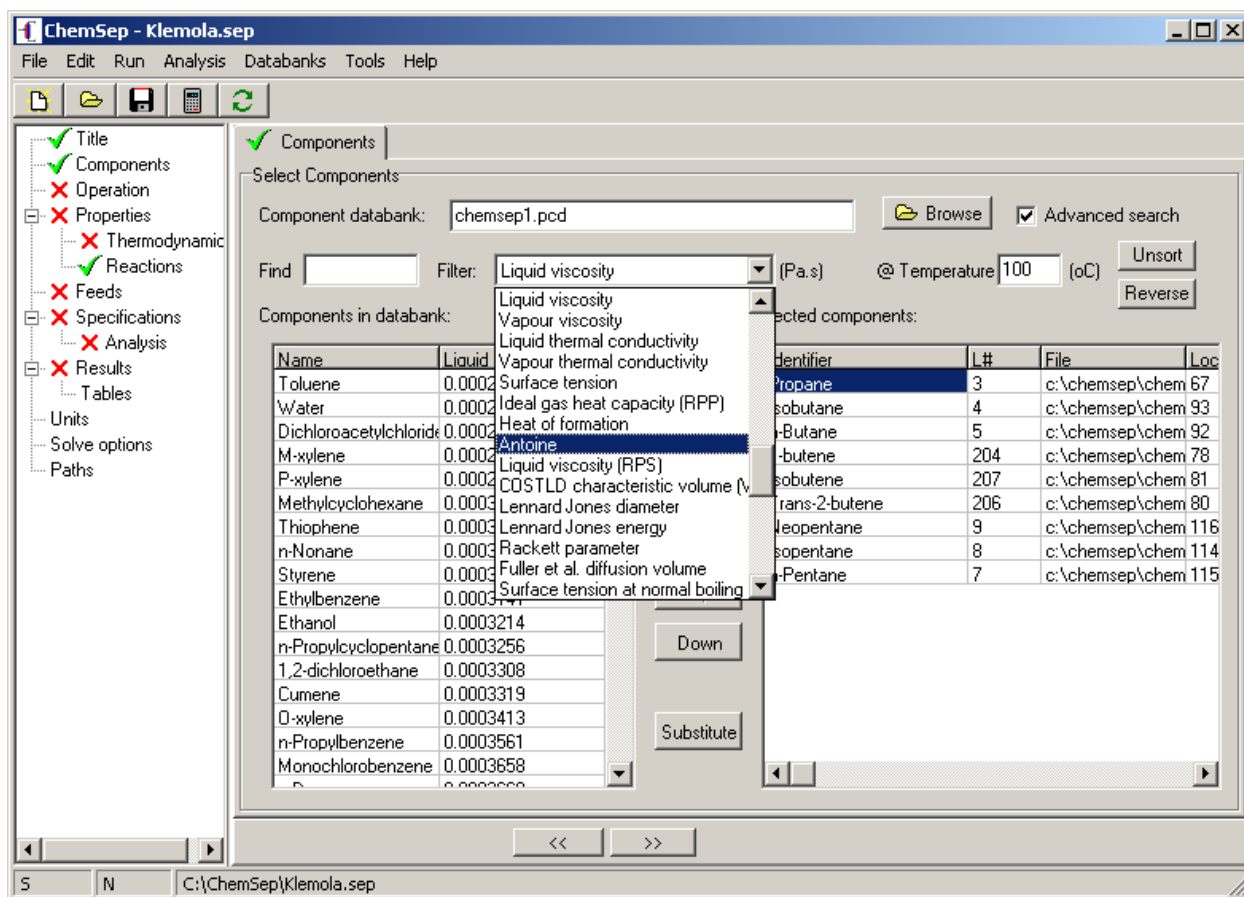
Graphical User Interface: New in Release 5.0 is a graphical user interface for Windows that retains much of the look and feel of the classic *ChemSep* interface. Problem solving is even easier with the new version however; new features make navigation within the interface much faster and the novice is taken through the problem solving process in a natural way. Input may include simple algebraic calculations as well as units. *ChemSep* checks your input, lets you know when each phase of problem setup is complete, and flags potential sources of difficulty before running a simulation.

Nonequilibrium column model: Taking the guesswork out of column simulation, *ChemSep* features a sophisticated nonequilibrium or rate-based model (Krishnamurthy and Taylor, 1985; Taylor and Krishna, 1993). The model in *ChemSep* includes the only available rate-based model for liquid-liquid extraction. The built in *Design Mode* allows the engineer to use proven rate-based technology in preliminary design. *ChemSep* features more column mass transfer coefficient correlations than any other similar model.



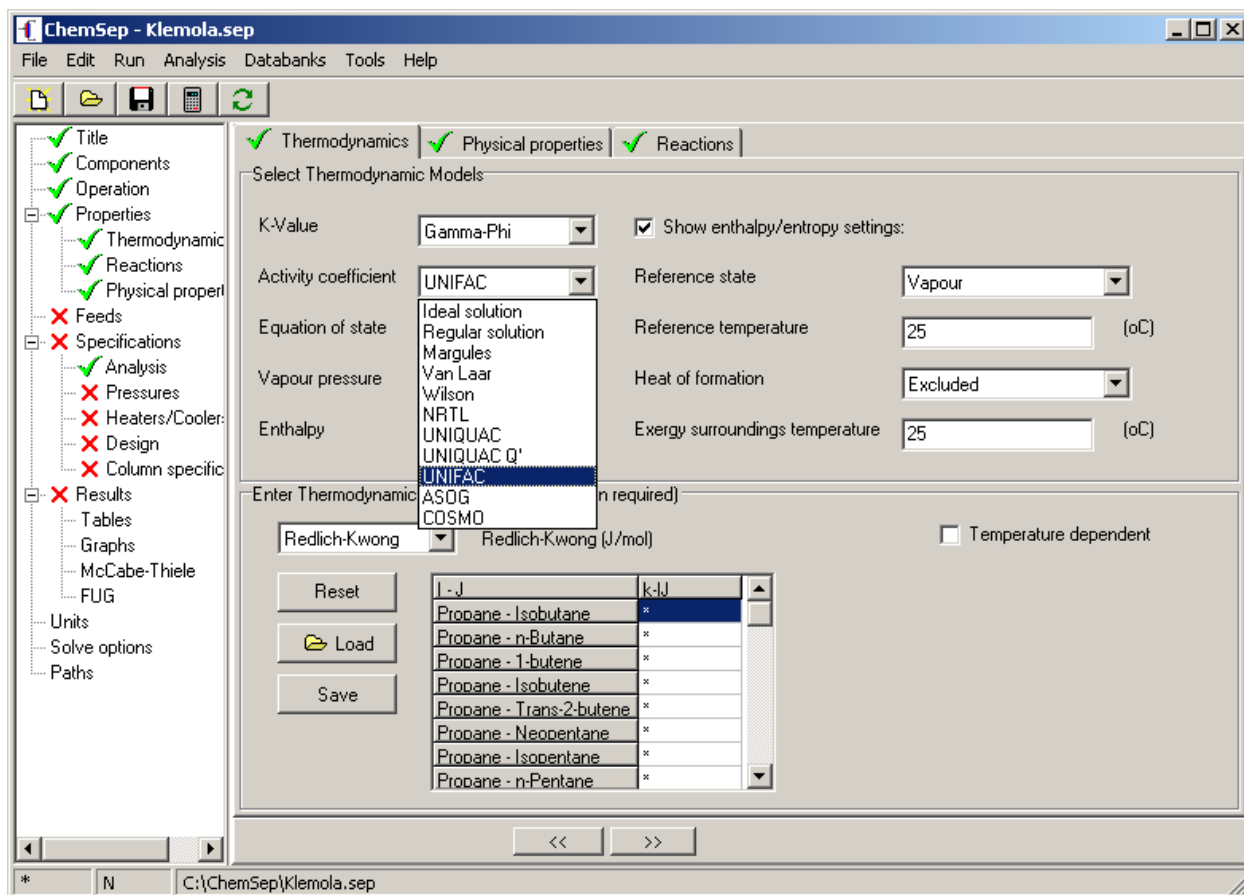
Most of the illustrations that accompany this article are based on our simulation with *ChemSep* of an industrial deisobutanizer described in detail by Klemola and Ilme (1996) and shown schematically above.

Databank: ChemSep comes with a databank of 189 common chemicals. Available at additional cost is a license to the industry standard DIPPR databank of over 1000 chemicals. Users can create their own libraries of physical property data. Selected components appear in the list on the right. The list can be re-ordered and components replaced at a later stage if so desired. If a text string is typed into the *Find* field the list shrinks to include only those components whose names include the text string. Chemical formula, structure, CAS number, or one of 50+ property values including temperature dependant properties can be used to select components. The illustration below shows component selection on the basis of their liquid viscosities at 100 Celcius. The advanced search capability is available only after clicking in the *Advanced Search* checkbox in the top right of the panel.



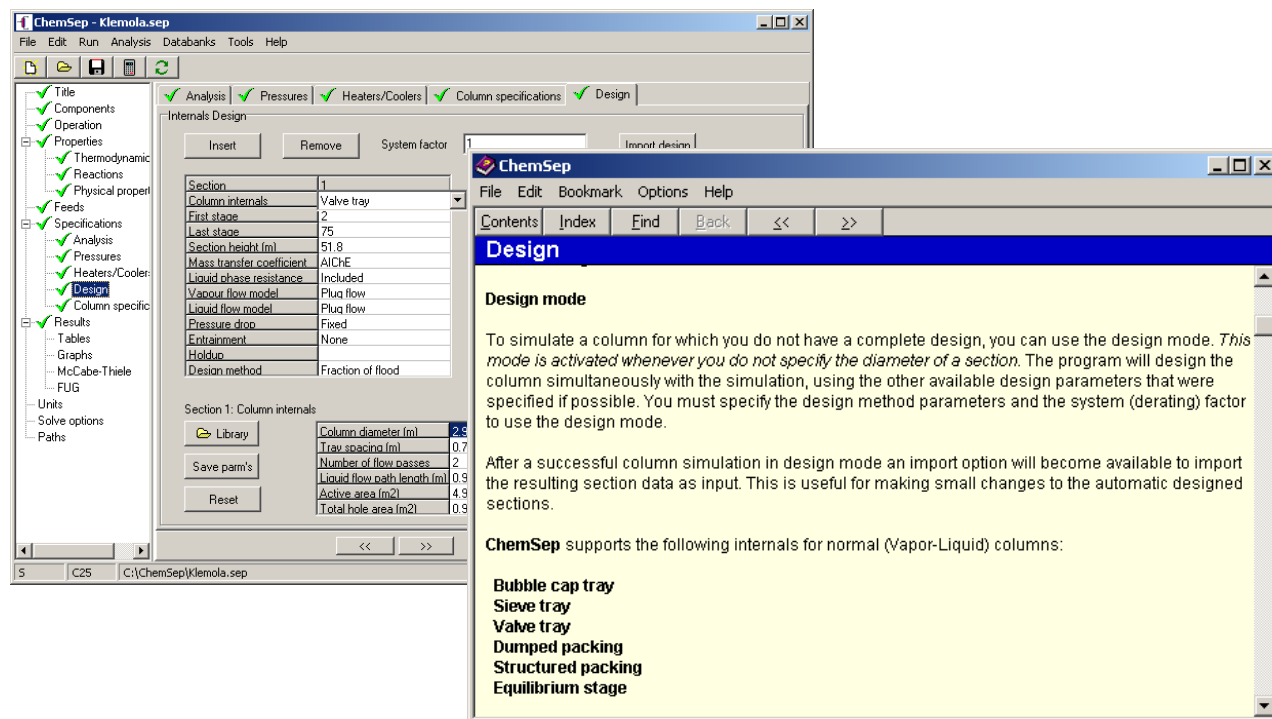
Components can be identified (see the first column of the selected components list on the lower right of the figure above) by their name, formula, or structural formula. It is also possible to simply type any desired text string to be used as the component label within the program.

Thermodynamic and Physical Property Models: ChemSep includes almost all of the most widely used thermodynamic models: 7 K-value models including DECHEMA (modified Raoult's law), Equation of State, and Chao-Seader; 10 Activity coefficient models including UNIFAC; and 8 equations of state including Peng-Robinson and Hayden-O'Connell (with chemical theory). ChemSep also includes a large number of physical property models (viscosity, thermal conductivity, surface tension, diffusivity) that are needed in nonequilibrium column modeling.



In this example (and following Klemola and Ilme, 1996) we used the Gamma-Phi approach with the UNIFAC model for liquid phase activity coefficients, the Antoine equation for the vapor pressures and the SRK equation of state for the vapor phase fugacity coefficients. The lower half of the panel remains blank until the user selects a model that requires parameters. Parameters can be typed in by the user or loaded from libraries. The * in the figures indicated that default values are assigned. For the SRK model shown here the default values are zero, for activity coefficient models ChemSep will use UNIFAC to estimate any missing parameters. The right hand half of the upper panel is normally blank until the user clicks in the checkbox at the top (as is done here so that the reference state for enthalpy and entropy calculations is displayed so that they can be changed if desired).

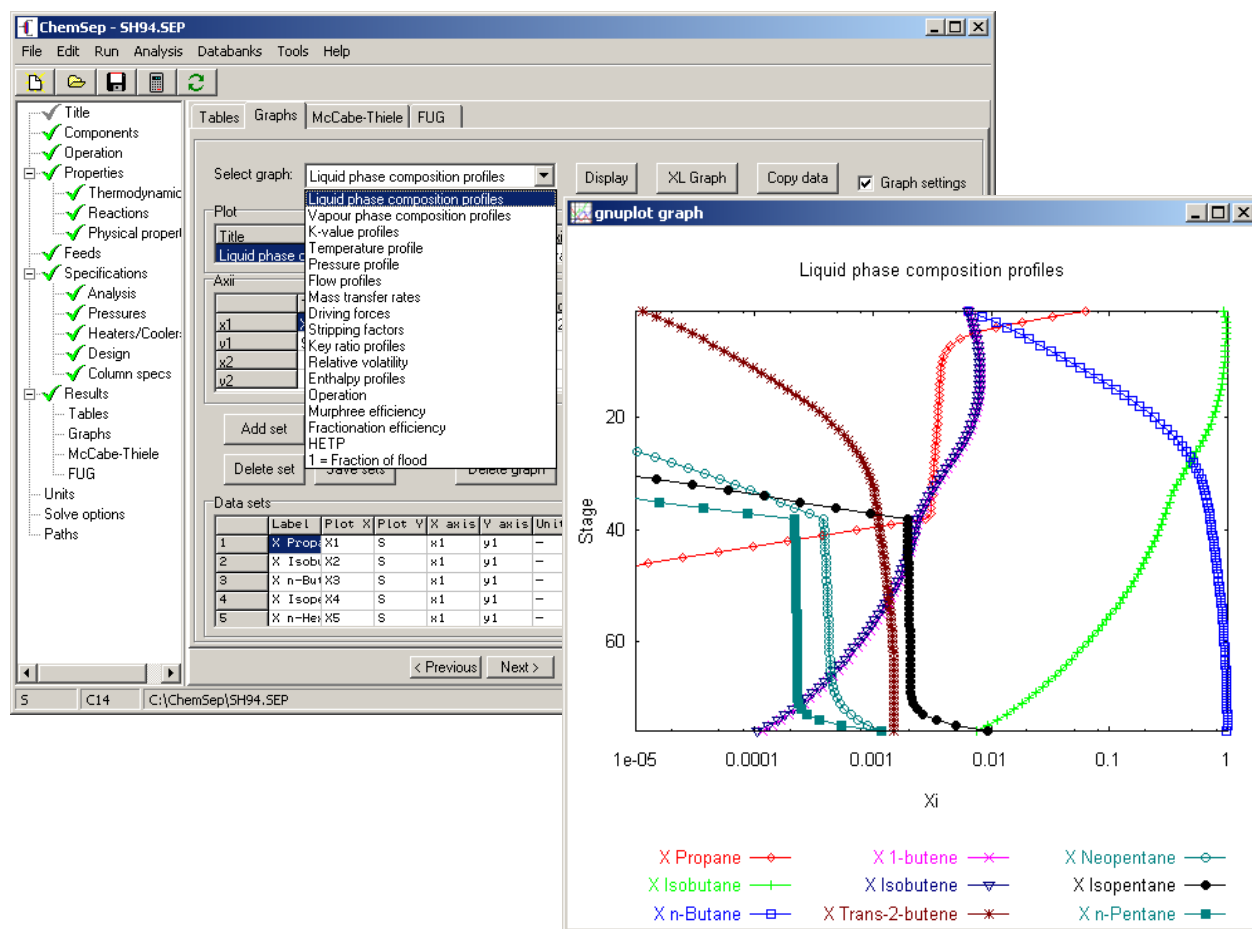
Column Design: For a nonequilibrium simulation we must say something about the type of column. Below is shown the design panel on which the equipment design details for the deisobutanizer are recorded and the help page that proffers advice for the perplexed. Locating the cursor on the field(s) on the top line (Column internals) brings up a pull down list from which the user selects the type of tray or packing (a single column can have many different types of internal; if desired). In addition, a spreadsheet appears at the bottom of the panel in which the design details for that section are recorded. If the diameter is left unspecified (denoted by a *) *ChemSep* enters design mode and the internals are sized during the simulation. *ChemSep* incorporates methods for the simultaneous design of many different kinds of column internal.



ChemSep includes over 40 correlations for mass transfer coefficients in different types of column, as well as 18 different ways to estimate pressure drop and 16 for holdup.

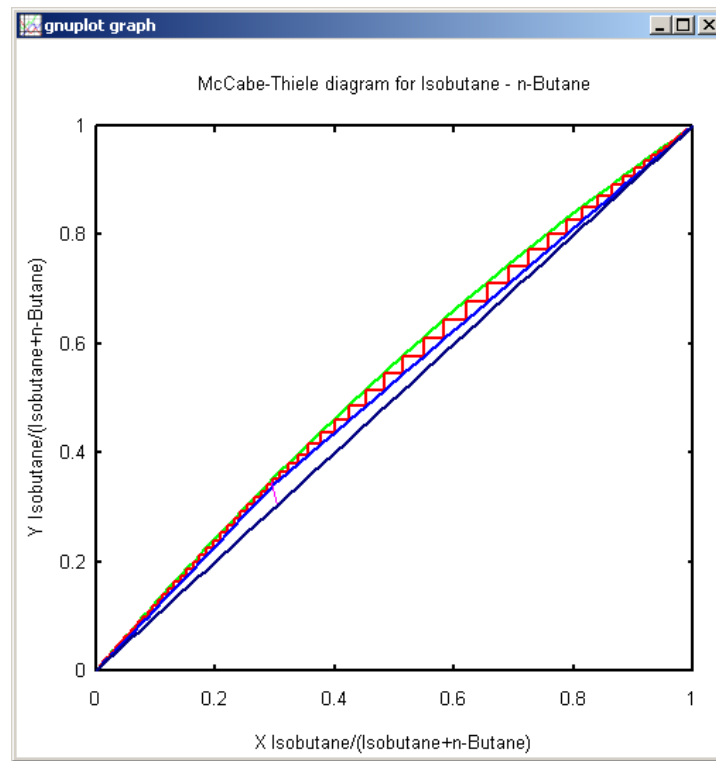
Degrees of Freedom Analysis: *ChemSep* tells you the number of degrees of freedom and identifies how many variables remain to be specified. When all degrees of freedom are satisfied *ChemSep* displays a green checkmark next to all input panels. While any degree of freedom remains to be satisfied *ChemSep* displays a large red X next to the input panels that require attention.

Powerful plotting capabilities: ChemSep has extensive support for plotting almost any kind of column profile including composition, flow, temperature, pressure, K-values, and more (see figure below). The plots are completely configurable. ChemSep uses the Open Source package Gnuplot (for Windows) to display a plot in its own separate window. Except where noted, the plots that appear in this article were created with Gnuplot and pasted directly into the word processor used to create this article. The illustration below shows graph selection in action and the resulting plot. The *Graph settings* checkbox (upper right) allows the user to configure the details of the graph before it is displayed.

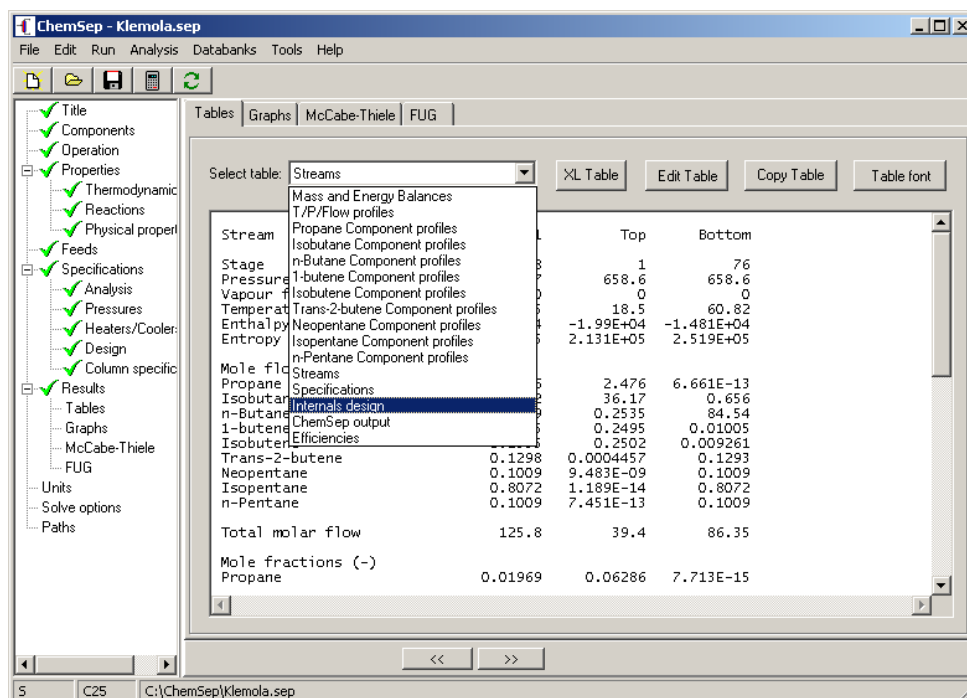


Users can design their own plots and include them in the pull-down plot selection list for future use. From the results of a nonequilibrium simulation one can plot profiles of any physical property as well as numerous design-related variables such as froth height in a tray column, approach to flooding, or specific interfacial area (these are just a few of many variables that can be plotted).

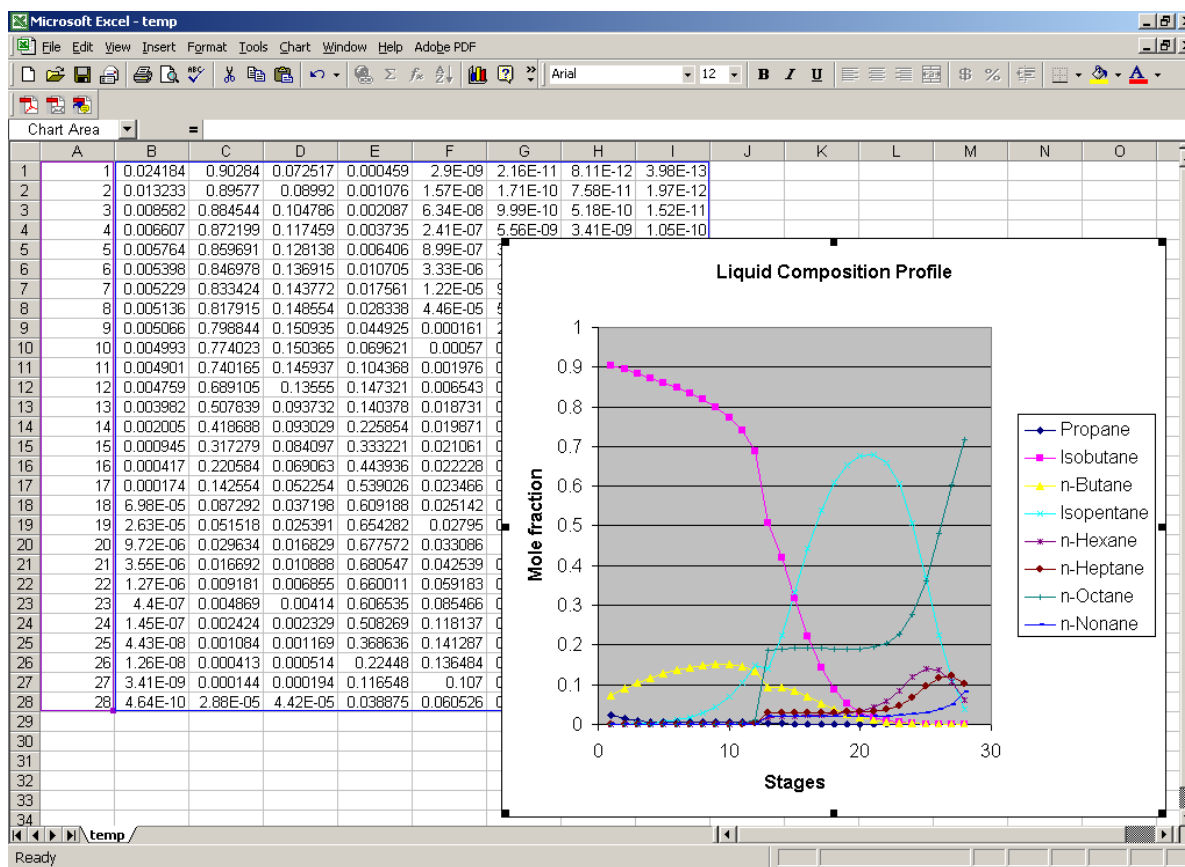
McCabe-Thiele Diagrams are a standard feature in *ChemSep* (even for multicomponent systems like the deisobutanizer).



Tabular Output can be viewed in *ChemSep*, or sent directly to text editor such as Notepad or spreadsheet program such as Excel.



Export: Simulation results may be saved in a variety of formats such as text, html and csv. Tables and graphs may be sent directly to Excel (see the buttons *XL Table* and *XL Graph* that sends the data directly to Excel where it can be plotted as shown below for an example from Seader and Henley (1998).



ChemSep-Lite Now Available for Nothing!

A version of *ChemSep* with limited functionality is available for free download from www.chemsep.org/downloads/index.html. That's right, no fee at all, not now, not ever! *ChemSep* Lite is limited to no more than four components, a databank with a limited number of components, no more than 50 stages in a column simulation, and no nonequilibrium model.

Whats Next?

In a subsequent release of *ChemSep* (tentatively scheduled for spring 2005) we plan to build in phase diagrams, property calculations and plots, and residue curve maps. In prior releases of *ChemSep* this functionality was available in the separate program ChemProp.

A CAPE OPEN compliant version will also be available in 2005.

Availability

ChemSep is available for educational use from the CACHE corporation (www.cache.org). For licenses for non-educational use please contact the authors.

Further Information

Additional information about the program can be found at www.chemsep.org. The authors can be contacted at kooijman@chemsep.org and taylor@chemsep.org.

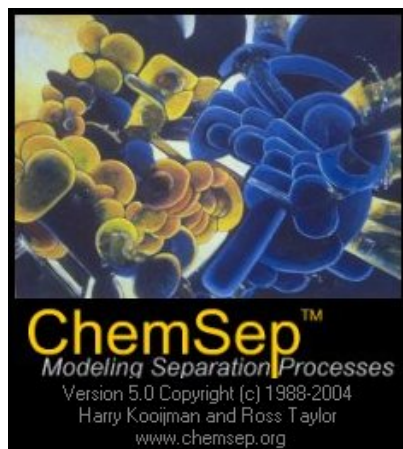
References and Further Reading

The books by Benitez and by Seader and Henley mention *ChemSep* and use it to solve some example problems.

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Final Note

The illustration shown below is the splash screen that is displayed on initial execution of *ChemSep*. The artwork is by Morris Bennett (MA). You can see more of his art at <http://www.chemsep.org/downloads/art/art.html>. Bennett writes:



My paintings are a combination of many different art styles synthesized with directly observed forms in nature. Music and other sounds are also among my influences. I exploit the human tendency to project inner states on outer forms by using my academic training to paint non-representational images.

Guided primarily by intuition, I create my paintings from all four edges, thus most of my work can be rotated to reveal completely different imagery.

My intention is to invite people to explore the worlds I have created and to come away with an increased, though not necessarily definable, understanding of reality.

Femlab 3.0: Experiences in Determining RTD

*Edward M. Rosen
EMR Technology Group*

Introduction

The use of commercially available Computational Fluid Dynamics (CFD) packages to study the residence time distribution (RTD) in wastewater treatment plants was recently discussed (Madeira, et. al , 2004). In that study the Fluent package (ver 6.0) (<http://www.fluent.com>) was used to simulate a 2-D reservoir with dimensions L (length) and H (height) in laminar flow and isothermal conditions (see Figure 1).

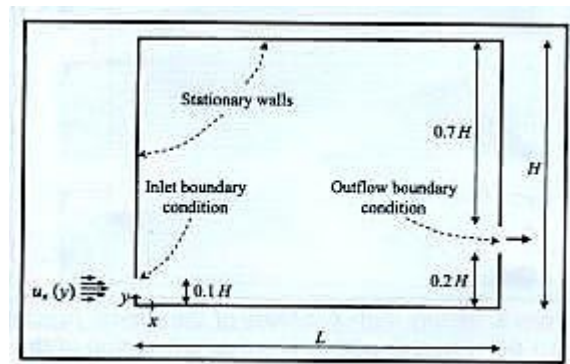


Figure 1 Sketch of Reservoir Geometry

(From Madeira et. al., 2004 with permission)¹

Both the inlet and the outlet boundaries of the reservoir have a height of 0.01 m with distances from the bottom of the reservoir of 0 and 0.02 m, respectively. Both L and H = 0.1 m.

A fully developed parabolic velocity profile is imposed on the inlet boundary

$$u_x = U_{max} [1 - \{(y-H/20)/H/20\}^2] \quad (1)$$

where

$$U_{max} = 1.5 \, U_{mean}$$

There is no slip at the walls ($u_x = u_y = 0$).

A step input of a component with properties similar to water ($\eta = 0.001 \text{ kg/(m-s)}$, $\rho = 1000 \text{ kg/m}^3$, with $D = 5\text{E-}10 \text{ m}^2/\text{s}$) and having constant concentration (1000 kg/m^3) across the inlet boundary is introduced at time zero.

Results of the Study with Fluent

Figures 2 and 3 indicate the results of the studies by Madeira et. al., 2004 at various Reynolds numbers with $L/H = 1$. They present a table showing the influence of Reynolds number on the mean residence time.

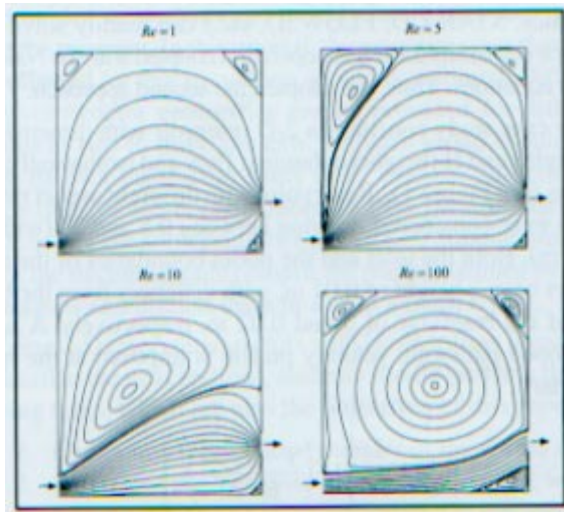


Figure 2. Steady state contours of the stream function for the reservoir with $L/H = 1$ as a function of Reynolds number

(From Madeira et. al., 2004 with permission)¹

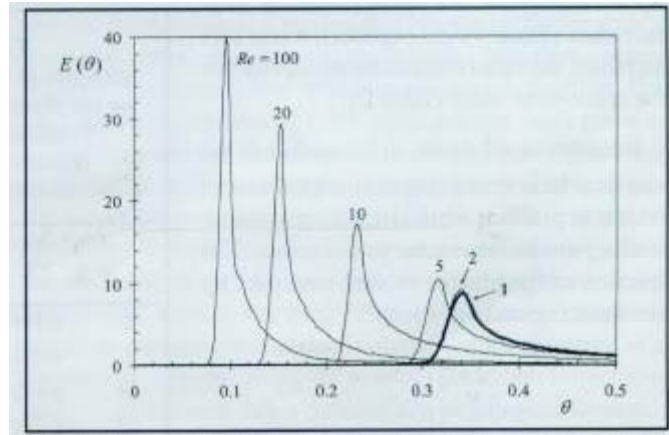


Figure 3 Effect of Reynolds number on the residence time distribution ($L/H = 1$)

(From Madeira et. al. 2004 with permission)¹

It is the purpose of this study to see how the same problem is solved using Femlab 3.0 (<http://www.comsol.com>). The study is limited to $Re = 10$ and $L/H = 1$.

Setting up Femlab

The general procedure followed using Femlab is:

1. Solve the ns (Navier-Stokes) equation at steady state
2. Solve the cd (Convection-Diffusion) equation starting at time zero to time 500 sec in time increments of 2 sec holding constant the steady state solution of the ns equation.
3. Record the integrated exit boundary concentration at the specified times on a spreadsheet for analysis of the RTD and mean residence time.

In Femlab Enter:

New, 2D

Chemical Engineering Module

Momentum Balance

Incompressible Navier-Stokes

Steady State Analysis (highlighted)

Click *Multiphysics* then *Add*

Mass Balance

Convection and Diffusion

Transient Analysis (highlighted)

Click *Add*

Click *OK*

Setting Up the Geometry

In Femlab enter with respect to Figure 1 ($H = 0.1$, $L = 0.1$):

Draw

Specify Objects

Line

Enter the line coordinates for each boundary of the geometry

Click on *Zoom Extents* (on the menu) after each line is entered.

Coerce to Solid

The inlet flow boundary is assigned as boundary 1, the outlet boundary is assigned as boundary 6, the top left boundary as 3, the top boundary as 4, the top right boundary as 7, the bottom right boundary as 5 and the bottom boundary as 2.

Setting up the Constants

In Femlab enter:

Options

Constants

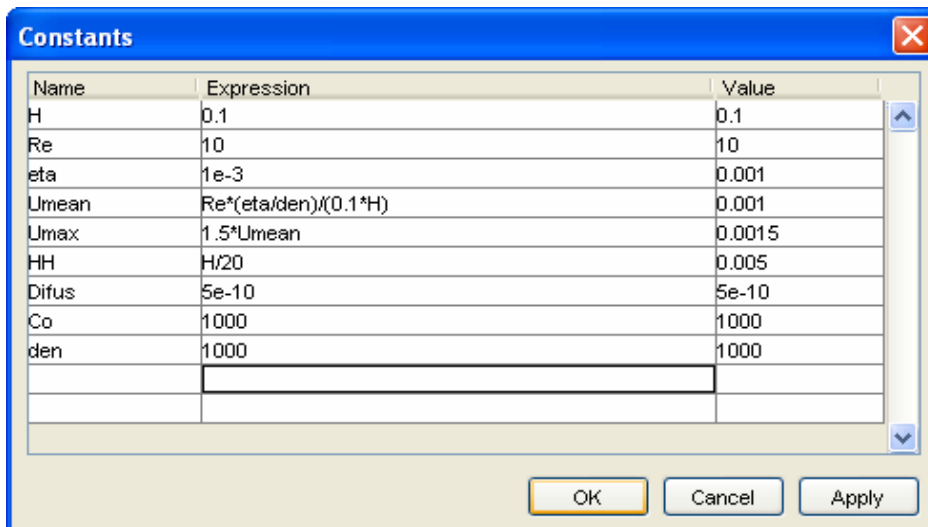


Figure 4. Femlab Constants window

Note (Figure 4) that $\eta = \eta$, $\rho = \rho$, Difus is D (the diffusivity) and Co is the concentration (kg/m^3) of the component at the inlet. τ is the space- time and U_{max} is calculated from the Reynolds number as shown.

Solving the Navier-Stokes Equations

In Femlab enter (*Multiphysics –ns*):

Options

Expressions

Boundary Expressions

Boundary Expression 1

Name	Expression
<i>uvel</i>	$U_{max} * [1 - ((y-HH)/HH)^2]$

Physics

Subdomain Settings 1

Physics Tab

ρ = den Density
 η = eta Dynamic Viscosity

Boundary Settings

Boundary Setting 1

Boundary Condition	Inflow/Outflow Velocity
$u_0 = uvel$	<i>x velocity</i>
$v_0 = 0$	<i>y velocity</i>

Boundary Setting 2

Boundary Condition No Slip

Boundary Setting 3

Boundary Condition No Slip

Boundary Setting 4

Boundary Condition No Slip

Boundary Setting 5

Boundary Condition No Slip

Boundary Setting 6

Boundary Condition OutFlow/ Pressure

Boundary Setting 7

Boundary Condition No Slip

Mesh

Initial Mesh

Refine Mesh

Refine Mesh

(A finer mesh size was tried but memory was found to be inadequate (512 MB)).

Solve

Solver Parameters

Stationary Nonlinear

Solver Manager

Initial Value Tab

Initial Value

Check Initial Value Expressions

Fixed Solution/Linearization Initialization Point

Check Initial Value

Solve for Tab

Geom 2D

Incompressible Navier-Stokes (highlight)

Output Tab

Geom 2D

Incompressible Navier-Stokes (highlight)

Solve Problem

Postprocessing

Plot Parameters

General Tab

Check Streamline

Streamline Tab

Check Number of Start Points (60)

Click OK

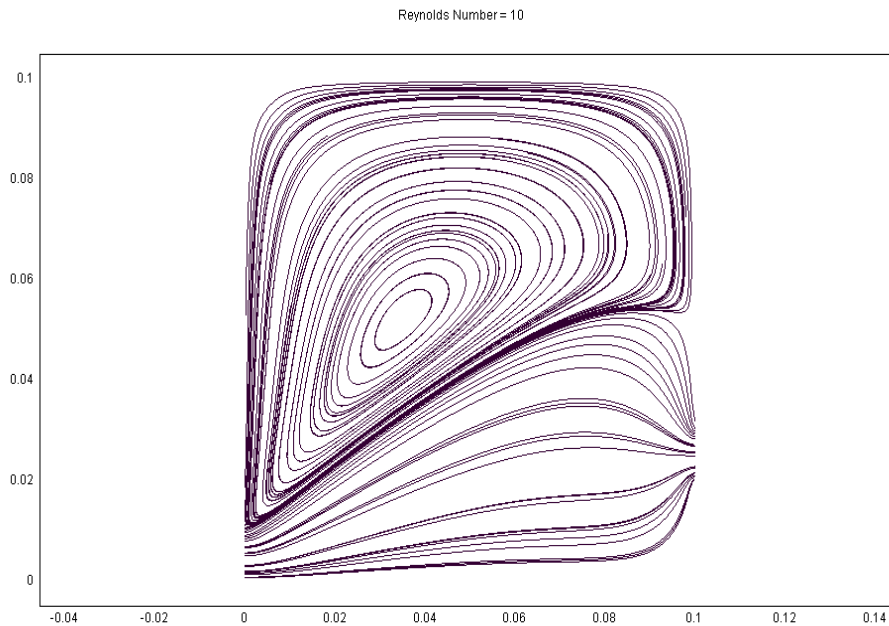


Figure 5 Streamlines of the solution at $Re = 10$

This output compares well to the Fluent results of Figure 2 at $Re = 10$.

Solving the Convection-Diffusion Equation

The solution to the time dependent convection-diffusion equation (cd) proved to require considerable trial and error since the problem is so convection dominant (Comsol_a, 2004). Femlab provides a number of artificial stabilization methods (Comsol_b, 2004) which modifies the original problem. Some of the methods, however, do not provide what were judged to be reasonable solutions.

When no stabilization is used, Figure 6 is the concentration profile that occurs after 222 sec. and Figure 7 is the results after 398 sec. A negative value for the integrated concentration at the exit at 222 sec is returned and the profile at 398 sec does not seem reasonable.

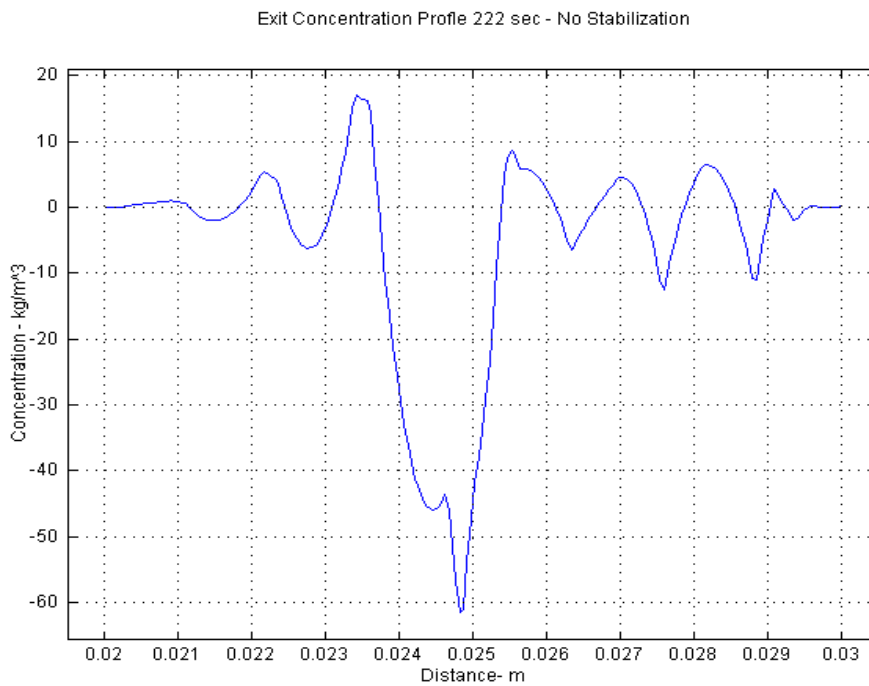


Figure 6. Exit concentration profile at 222 sec with no stabilization

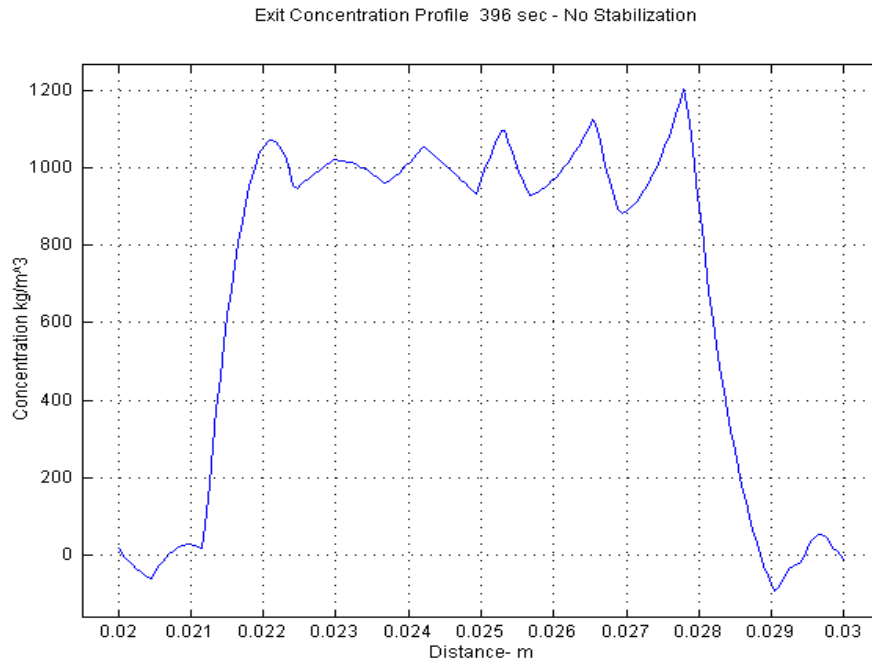


Figure 7 Exit Concentration Profile at 398 sec – No stabilization

Both streamline diffusion and crosswind diffusion stabilization methods were tried but rejected. Isotropic diffusion was most extensively tested and was finally accepted. The tuning parameter was slowly decreased from a value of 0.5 to 0.008, the point at which the concentration profiles were still acceptable (Figures 8 and 9).

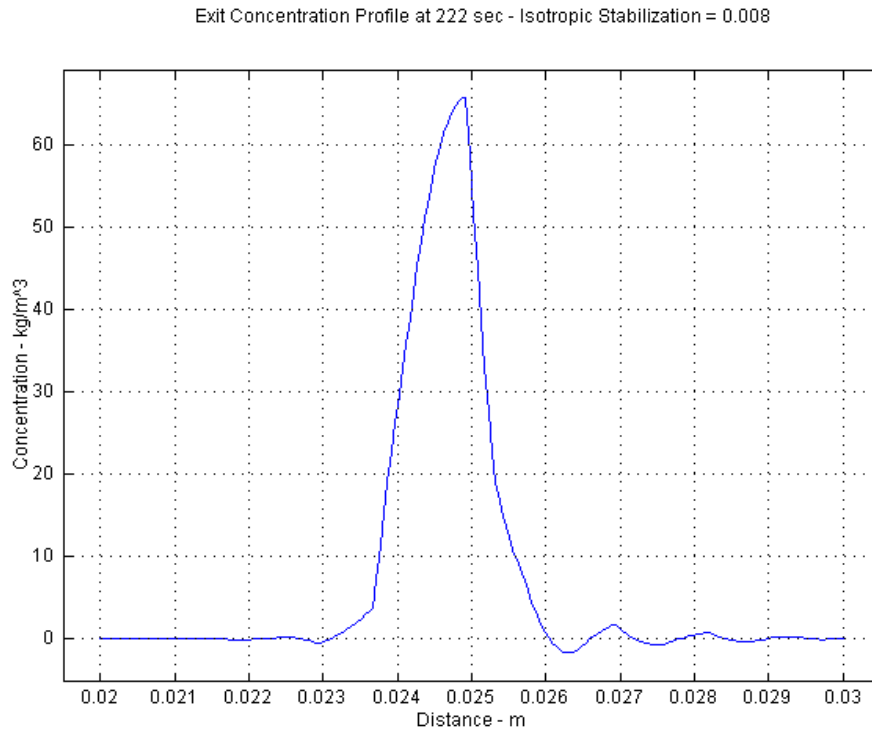


Figure 8 Exit concentration profile at 222 sec with isotropic stabilization = 0.008

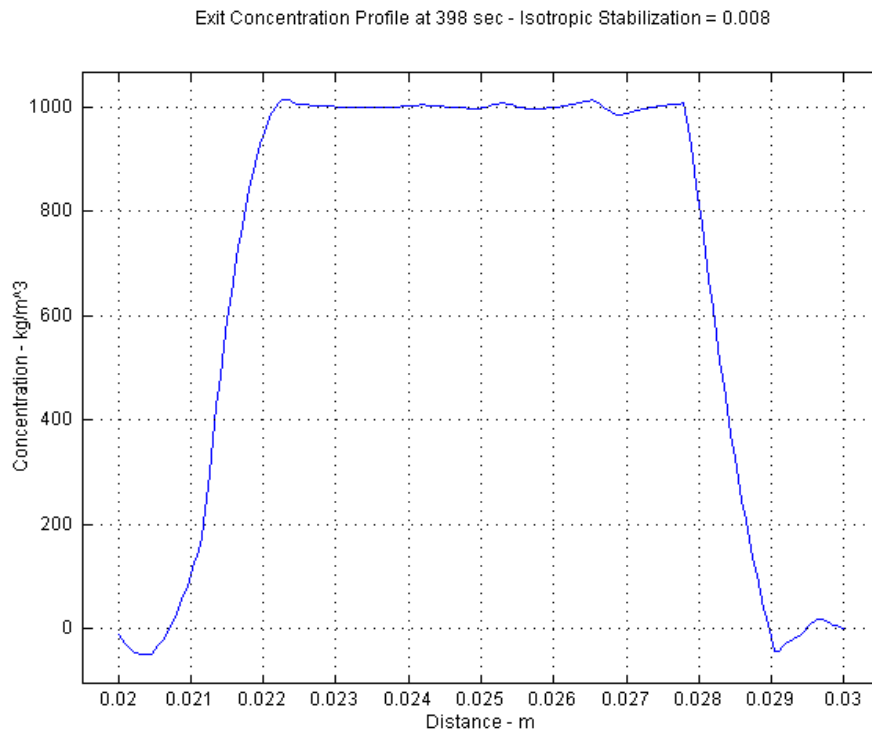


Figure 9 Exit Concentration Profile at 398 sec with isotropic stabilization= 0.008

The procedure with isotropic stabilization to solve the cd equation (storing the steady state ns solution):

Enter Femlab:

Multiphysics

Convection and Diffusion (highlighted)

Physics

Boundary Settings

<i>Boundary Selection</i>	<i>1</i>	<i>Concentration</i>
		<i>Co = Co</i>
<i>Boundary Selection</i>	<i>2</i>	<i>Insulation/Symmetry</i>
<i>Boundary Selection</i>	<i>3</i>	<i>Insulation/Symmetry</i>
<i>Boundary Selection</i>	<i>4</i>	<i>Insulation/Symmetry</i>
<i>Boundary Selection</i>	<i>5</i>	<i>Insulation/Symmetry</i>
<i>Boundary Selection</i>	<i>6</i>	<i>Convective Flux</i>
<i>Boundary Selection</i>	<i>7</i>	<i>Insulation Symmetry</i>

Subdomain Settings

c Tab

<i>D Isotropic</i>	<i>Difus</i>	<i>Diffusion Coeffiscient</i>
<i>u</i>	<i>u</i>	<i>x velocity</i>
<i>v</i>	<i>v</i>	<i>y velcity</i>

Artificial Diffusion

isotropic diffusion $\delta_{id} = 0.008$ Tuning Parameter

Init Tab

c(t_o) 0 Concentration c

Solve

Solver Parameters

General Tab

Solver – Time Dependent

Time Stepping – Time 0:2:500

Time Stepping Tab

Time step taken by Solver – Strict

Some differences were noted in how the time steps were determined (fixed, free) but the differences were not judged to be significant.

Solver Manager

Click *Store Solution*

Initial Value Tab

Initial Value

Click *Initial value expression evaluated using stored solution*

Fixed solution/Linearization point

Click *Stored Solution*

Solve for Tab

Geom(2D)

Convection and Diffusion (highlight)

Output Tab

Geom 2D

Incompressible Navier-Stokes (highlight)

Convection and Diffusion (highlight)

Solve

Click *Solve Problem*

Time of Solution : 677.9 sec Degrees of Freedom 100, 088

Postprocessing

The solution to the steady state ns equation and the transient cd equation can be viewed in a number of ways in the postprocessing step. Figure 10 shows the concentration of the tracer after 222 sec at which point the tracer is just reaching the exit. This is consistent with a similar plot presented by Maderia et. al., 2004.

Enter Femlab:

Postprocessing

General Tab

Check *Surface*

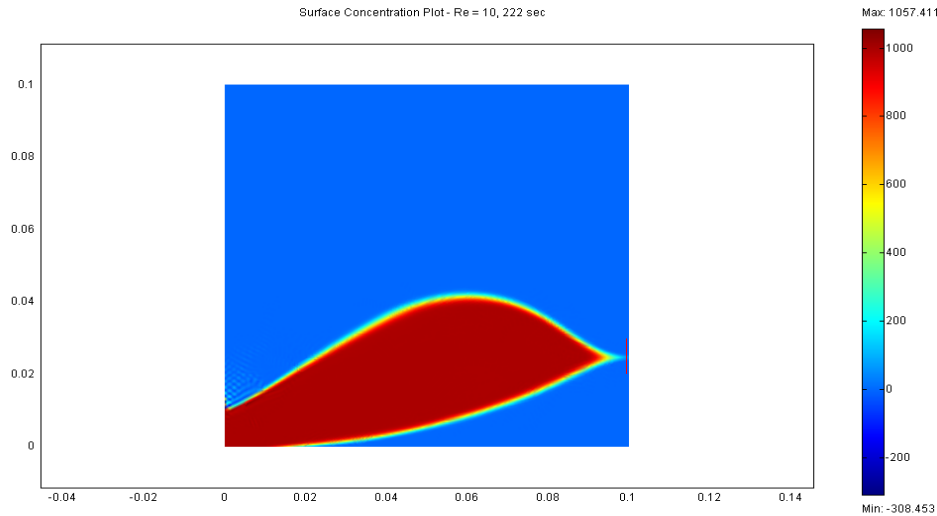


Figure 10 Surface tracer concentration for the reservoir after 222 sec
($Re = 10$, $L/H = 1$)

The cross sectional plots of Figures 6, 7, 8 and 9 were obtained at $x = 0.0995$ m ($y = 0.02$ to 0.03) rather than at $x = 0.1$ since a bug exists in Version 3.0 (Comsol_c, 2004).

Enter Femlab:

Postprocessing
Cross Sectional Plots
General (time selected)
Line Extension (cross section line data)

Spreadsheet Calculations

After the calculation for the cd equation is complete, postprocessing is accessed and boundary integration is requested:

Enter Femlab:

Postprocessing
Boundary Integration
Boundary Selection 6
Time (selected)

The integrated concentration at boundary 6 (the exit) is returned on the screen at the requested time and is entered manually into the spreadsheet (Appendix A) column 'Cout/Integrated'. The Danckwert's F curve values ($C_{out}/(0.01 \cdot C_o)$) are calculated in the next column where the 0.01 term is the height of the exit.

The resident-time distribution function

$$E(t) = d(F(t))/dt \quad (2)$$

is calculated using an average of the forward and backward derivative of the $F(t)$ values at a particular time (Chapra et al, 1988). Normalizing

$$E(\theta) = E(t)/\tau \quad (3)$$

where the space-time is

$$\tau = \text{Area} / \text{Flow Rate} = (0.1)*(0.1)/(.001*.01) = 1000 \text{ (1/s)} \quad (4)$$

Figure 11 is a plot of the residence time distribution ($E(\theta)$ vs θ) out to $\theta = 0.398$. The plot closely matches the results of Madeira et. al., 2004 except that the tail becomes unstable (compare Figure 3).

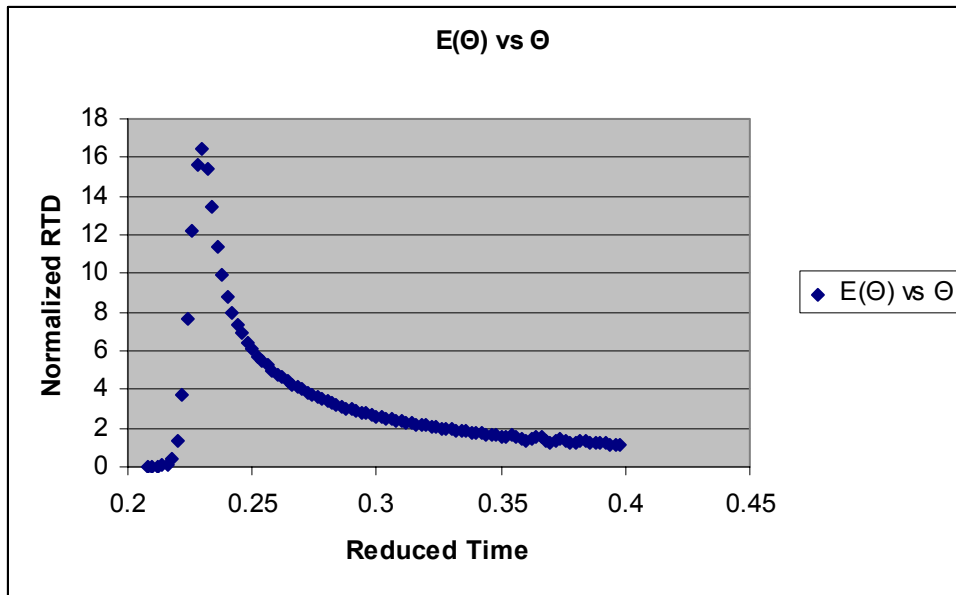


Figure 11 Residence time distribution for $Re = 10$, $L/H = 1$

Determination of Reduced Mean Residence Time

The mean reduced residence time $\bar{\theta}_r$ is given (Himmelblau et. al. 1968) by

$$\bar{\theta}_r = \bar{t}_r / \tau = \int_0^{\infty} \theta E(\theta) d\theta \quad (5)$$

where

$$\bar{t}_r = \int_0^{\infty} t E(t) dt \quad (6)$$

Since the tail of the RTD was unstable, determination of the area under the curve was broken into two parts: from $\theta = 0.208$ to $\theta = 0.398$ and from $\theta = 0.398$ to ∞ . The area of the first part of the curve was determined by using the trapezoidal rule (Appendix A). The trapezoidal rule was also used for the $\theta^* E(\theta)$ curve.

A plot of $\ln(E(\theta))$ vs θ is shown in Figure 12.

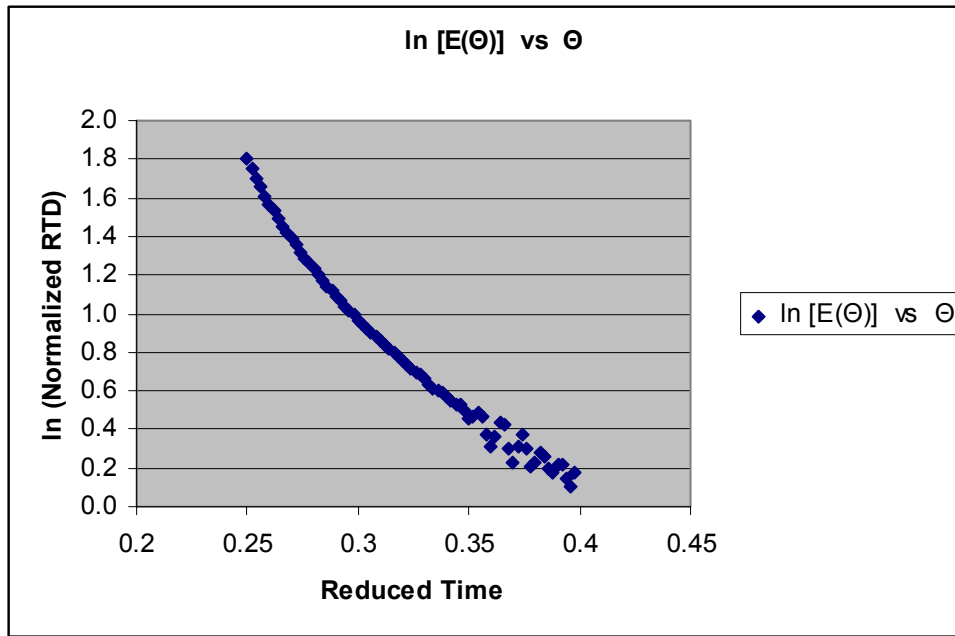


Figure 12. Plot of $\ln(E(\theta))$ vs θ

The plot indicates that a curve of the form

$$E(\theta) = A \exp(-B * \theta) \quad (7)$$

could approximate the tail of the curve from θ from 0.398 to ∞ .

The areas of both the $E(\theta)$ and $\theta * E(\theta)$ curve can then be calculated analytically from the following:

Noting that

$$\int_0^{\infty} E(\theta) d\theta = 1 \quad (8)$$

the area under the curve from $\theta = 0.398$ to ∞ must be $1 - 0.6590 = 0.3410$
where the 0.6590 is the area from $\theta = 0.208$ to 0.398

From Equation (7)

$$\int_{0.398}^{\infty} A \exp(-B * \theta) d\theta = (A/B) \exp(-B * 0.398) = 0.3410 \quad (9)$$

From the spreadsheet at $\theta = 0.398$

$$E(\theta) = 1.1875 = A \exp(-B * 0.398) \quad (10)$$

Using Equations (9) and (10)

$$B = 1.1875 / 0.3410 = 3.48240 \quad (11)$$

and from Equation (7)

$$A = 1.1875 / \exp(-3.48240 * 0.398) = 4.748579 \quad (12)$$

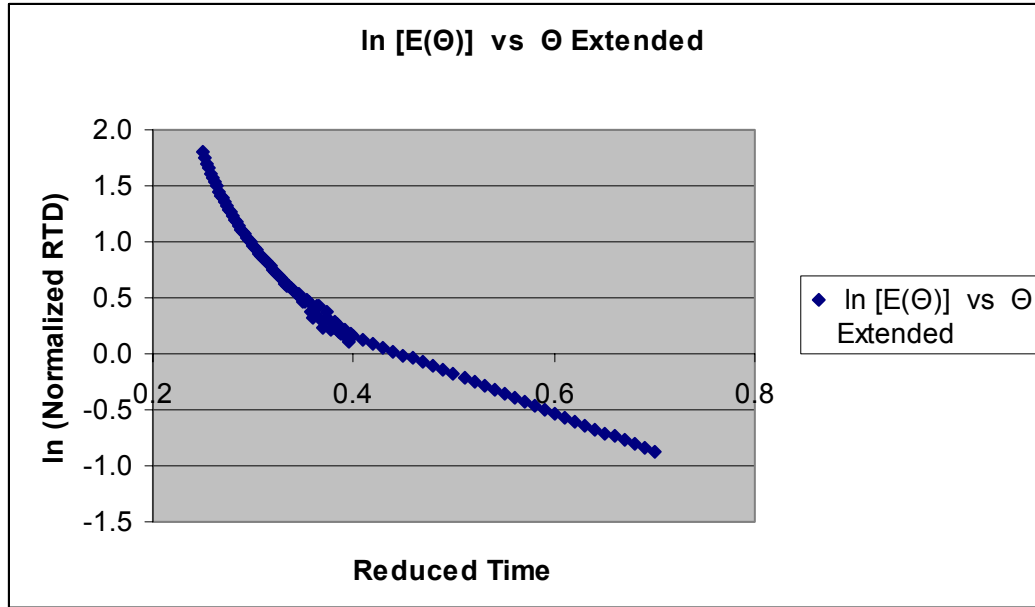


Figure 13 Plot of $\ln E(\theta)$ vs θ with approximate tail added

With the values of A and B available the tail of the $\theta * E(\theta)$ curve can be calculated analytically using equation (7):

$$\int_{.398}^{\infty} \theta E(\theta) d\theta = (A/B^2) * [(\exp(-0.398*B) * (-B(.398)-1))] = 0.2337 \quad (13)$$

When the tail value is added to the value of the integral calculated in the spreadsheet

$$\text{Total area under } \theta * E(\theta) \text{ curve} = 0.1798 + 0.2337 = \mathbf{0.4135} \quad (14)$$

This compares very well with the value of the mean residence time given by Madeira et al, 2004 of **0.412**.

Conclusions

The solution presented in this study is reasonable but could no doubt be improved. The solution presented by Madeira et. al., 2004. (Figure 2) did not appear to require any special processing for the tail and subsequent determination of the mean residence time by integration up to $\theta = 10$. Such a smooth tail could not be generated in this study using the application software.

Madeira et. al., 2004 did mention, however, that a special discretization scheme (Versteeg et. al, 1995) was used for the convective terms.

Madiera et. al., 2004 states “We must point out that to achieve a high level of accuracy, all the simulation results presented in his paper involved a detailed analysis of the numerical algorithms, the mesh employed, and the time step adopted (in transient simulations)” . A similar statement can perhaps be made with regard to Femlab 3.0.

Nomenclature

A, B	Parameters in Eq 7
C	Concentration (kg/m ³)
d	Inlet boundary height (m)
D	Diffusivity (m ² /s)
E(t)	Resident-time distribution function
E(θ)	Normalized RTD function, dimensionless
F(t)	Danckwerts' F curve, dimensionless
H	Height of reservoir, (m)
HH	= H/20
L	Length of reservoir, (m)
Q	Flow rate (m ² /s)
Re	Reynolds number, $dU_{\text{mean}}\rho/\eta$
t	Time (s)
\bar{t}_r	mean residence time (s)
Umax	fluid velocity at the center of the inlet boundary (m/s)
Umean	mean fluid velocity at the inlet boundary (m/s)
u _x	x-velocity (m/s)
u _y	y-velocity (m/s)
x	horizontal coordinate (m)
y	vertical coordinate (m)

Greek Symbols

δ_{id}	isotropic diffusion tuning parameter
η	dynamic viscosity (kg/m-s)
θ	$= t/\tau$, reduced time, dimensionless
$\bar{\theta}_r$	reduced mean residence time, dimensionless
ρ	density (kg/m ³)
τ	space-time (s)

References

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2. Comsol_a, Technical Support, e-mail of 8/27/2004, Case 29001
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6. Himmelblau, D. M. and K. B. Bischoff, *Process Analysis and Simulation*, John Wiley, New York (1968)
7. Versee, H. K. and W. Malalasekera, *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*, Prentice Hall, New Jersey (1995)

Acknowledgement:

The comments of Prof. P. Rony and the comments and help from technical support of Comsol Inc. is appreciated.

Appendix A – The Spreadsheet

Residence Time Calculations - CEE Spring 2004 p154

	τ	1000	δ_{id}	0.008			
	C_0	1000					
Time sec	$\theta = t/\tau$	Cout Integrated	F(t) = Cout/(0.01* C_0)	E(t)	E(θ)	$\theta^* E(\theta)$	ln [$E(\theta)$]
206	0.206	1.078E-05	1.078E-06				
208	0.208	2.080E-05	2.080E-06	1.700E-06	0.00170	0.00035	-6.3772
210	0.21	7.877E-05	7.877E-06	2.899E-06	0.00290	0.00061	-5.8435
212	0.212	1.368E-04	1.368E-05	1.840E-05	0.01840	0.00390	-3.9955
214	0.214	8.147E-04	8.147E-05	5.508E-05	0.05508	0.01179	-2.8989
216	0.216	2.340E-03	2.340E-04	1.210E-04	0.12098	0.02613	-2.1121
218	0.218	5.654E-03	5.654E-04	3.826E-04	0.38263	0.08341	-0.9607
220	0.22	1.765E-02	1.765E-03	1.347E-03	1.34713	0.29637	0.2980
222	0.222	5.954E-02	5.954E-03	3.695E-03	3.69452	0.82018	1.3068
224	0.224	1.654E-01	1.654E-02	7.641E-03	7.64070	1.71152	2.0335
226	0.226	3.652E-01	3.652E-02	1.224E-02	12.23534	2.76519	2.5043
228	0.228	6.548E-01	6.548E-02	1.566E-02	15.65590	3.56955	2.7508
230	0.23	9.914E-01	9.914E-02	1.643E-02	16.42785	3.77841	2.7990
232	0.232	1.312E+00	1.312E-01	1.538E-02	15.38010	3.56818	2.7331
234	0.234	1.607E+00	1.607E-01	1.345E-02	13.44752	3.14672	2.5988
236	0.236	1.850E+00	1.850E-01	1.134E-02	11.34020	2.67629	2.4284
238	0.238	2.060E+00	2.060E-01	9.909E-03	9.90938	2.35843	2.2935
240	0.24	2.246E+00	2.246E-01	8.823E-03	8.82328	2.11759	2.1774
242	0.242	2.413E+00	2.413E-01	7.991E-03	7.99125	1.93388	2.0783
244	0.244	2.566E+00	2.566E-01	7.376E-03	7.37608	1.79976	1.9982
246	0.246	2.708E+00	2.708E-01	6.891E-03	6.89125	1.69525	1.9303
248	0.248	2.842E+00	2.842E-01	6.450E-03	6.45040	1.59970	1.8641
250	0.25	2.966E+00	2.966E-01	6.055E-03	6.05493	1.51373	1.8009
252	0.252	3.084E+00	3.084E-01	5.739E-03	5.73918	1.44627	1.7473
254	0.254	3.196E+00	3.196E-01	5.483E-03	5.48285	1.39264	1.7016
256	0.256	3.303E+00	3.303E-01	5.240E-03	5.24008	1.34146	1.6563
258	0.258	3.405E+00	3.405E-01	5.004E-03	5.00420	1.29108	1.6103
260	0.26	3.503E+00	3.503E-01	4.799E-03	4.79877	1.24768	1.5684
262	0.262	3.597E+00	3.597E-01	4.621E-03	4.62140	1.21081	1.5307
264	0.264	3.688E+00	3.688E-01	4.450E-03	4.45025	1.17487	1.4930
266	0.266	3.775E+00	3.775E-01	4.283E-03	4.28338	1.13938	1.4547
268	0.268	3.859E+00	3.859E-01	4.131E-03	4.13083	1.10706	1.4185
270	0.27	3.941E+00	3.941E-01	3.996E-03	3.99645	1.07904	1.3854
272	0.272	4.019E+00	4.019E-01	3.871E-03	3.87098	1.05291	1.3535
274	0.274	4.095E+00	4.095E-01	3.747E-03	3.74725	1.02675	1.3210
276	0.276	4.169E+00	4.169E-01	3.633E-03	3.63333	1.00280	1.2901
278	0.278	4.241E+00	4.241E-01	3.532E-03	3.53185	0.98185	1.2618
280	0.28	4.310E+00	4.310E-01	3.434E-03	3.43363	0.96141	1.2336
282	0.282	4.378E+00	4.378E-01	3.330E-03	3.33040	0.93917	1.2031

284	0.284	4.444E+00	4.444E-01	3.228E-03	3.22755	0.91662	1.1717
286	0.286	4.507E+00	4.507E-01	3.133E-03	3.13268	0.89595	1.1419
288	0.288	4.569E+00	4.569E-01	3.048E-03	3.04792	0.87780	1.1145
290	0.29	4.629E+00	4.629E-01	2.971E-03	2.97147	0.86173	1.0891
292	0.292	4.688E+00	4.688E-01	2.900E-03	2.90005	0.84681	1.0647
294	0.294	4.745E+00	4.745E-01	2.831E-03	2.83093	0.83229	1.0406
296	0.296	4.801E+00	4.801E-01	2.763E-03	2.76260	0.81773	1.0162
298	0.298	4.856E+00	4.856E-01	2.695E-03	2.69540	0.80323	0.9915
300	0.3	4.909E+00	4.909E-01	2.631E-03	2.63083	0.78925	0.9673
302	0.302	4.961E+00	4.961E-01	2.570E-03	2.57037	0.77625	0.9441
304	0.304	5.012E+00	5.012E-01	2.515E-03	2.51450	0.76441	0.9221
306	0.306	5.061E+00	5.061E-01	2.462E-03	2.46188	0.75333	0.9009
308	0.308	5.110E+00	5.110E-01	2.410E-03	2.41037	0.74240	0.8798
310	0.31	5.158E+00	5.158E-01	2.359E-03	2.35890	0.73126	0.8582
312	0.312	5.205E+00	5.205E-01	2.309E-03	2.30850	0.72025	0.8366
314	0.314	5.250E+00	5.250E-01	2.261E-03	2.26130	0.71005	0.8159
316	0.316	5.295E+00	5.295E-01	2.218E-03	2.21815	0.70094	0.7967
318	0.318	5.339E+00	5.339E-01	2.177E-03	2.17658	0.69215	0.7778
320	0.32	5.382E+00	5.382E-01	2.133E-03	2.13280	0.68250	0.7574
322	0.322	5.424E+00	5.424E-01	2.087E-03	2.08695	0.67200	0.7357
324	0.324	5.465E+00	5.465E-01	2.044E-03	2.04403	0.66226	0.7149
326	0.326	5.506E+00	5.506E-01	2.008E-03	2.00773	0.65452	0.6970
328	0.328	5.546E+00	5.546E-01	1.973E-03	1.97333	0.64725	0.6797
330	0.33	5.585E+00	5.585E-01	1.931E-03	1.93140	0.63736	0.6582
332	0.332	5.623E+00	5.623E-01	1.882E-03	1.88242	0.62497	0.6326
334	0.334	5.660E+00	5.660E-01	1.842E-03	1.84200	0.61523	0.6109
336	0.336	5.697E+00	5.697E-01	1.822E-03	1.82203	0.61220	0.5999
338	0.338	5.733E+00	5.733E-01	1.809E-03	1.80862	0.61132	0.5926
340	0.34	5.769E+00	5.769E-01	1.775E-03	1.77522	0.60358	0.5739
342	0.342	5.804E+00	5.804E-01	1.726E-03	1.72580	0.59022	0.5457
344	0.344	5.838E+00	5.838E-01	1.702E-03	1.70238	0.58562	0.5320
346	0.346	5.872E+00	5.872E-01	1.699E-03	1.69860	0.58772	0.5298
348	0.348	5.906E+00	5.906E-01	1.647E-03	1.64728	0.57325	0.4991
350	0.35	5.938E+00	5.938E-01	1.579E-03	1.57925	0.55274	0.4570
352	0.352	5.969E+00	5.969E-01	1.588E-03	1.58815	0.55903	0.4626
354	0.354	6.002E+00	6.002E-01	1.628E-03	1.62758	0.57616	0.4871
356	0.356	6.034E+00	6.034E-01	1.587E-03	1.58707	0.56500	0.4619
358	0.358	6.065E+00	6.065E-01	1.453E-03	1.45287	0.52013	0.3735
360	0.36	6.092E+00	6.092E-01	1.368E-03	1.36808	0.49251	0.3134
362	0.362	6.120E+00	6.120E-01	1.440E-03	1.44010	0.52132	0.3647
364	0.364	6.150E+00	6.150E-01	1.549E-03	1.54875	0.56374	0.4374
366	0.366	6.182E+00	6.182E-01	1.525E-03	1.52530	0.55826	0.4222
368	0.368	6.211E+00	6.211E-01	1.351E-03	1.35118	0.49723	0.3010
370	0.37	6.236E+00	6.236E-01	1.258E-03	1.25775	0.46537	0.2293
372	0.372	6.261E+00	6.261E-01	1.361E-03	1.36143	0.50645	0.3085
374	0.374	6.290E+00	6.290E-01	1.447E-03	1.44725	0.54127	0.3697
376	0.376	6.319E+00	6.319E-01	1.355E-03	1.35513	0.50953	0.3039
378	0.378	6.344E+00	6.344E-01	1.236E-03	1.23558	0.46705	0.2115
380	0.38	6.369E+00	6.369E-01	1.258E-03	1.25765	0.47791	0.2292
382	0.382	6.395E+00	6.395E-01	1.326E-03	1.32632	0.50666	0.2824
384	0.384	6.422E+00	6.422E-01	1.299E-03	1.29947	0.49900	0.2620
386	0.386	6.447E+00	6.447E-01	1.216E-03	1.21573	0.46927	0.1953

388	0.388	6.470E+00	6.470E-01	1.196E-03	1.19592	0.46402	0.1789
390	0.39	6.495E+00	6.495E-01	1.245E-03	1.24530	0.48567	0.2194
392	0.392	6.520E+00	6.520E-01	1.246E-03	1.24578	0.48834	0.2198
394	0.394	6.544E+00	6.544E-01	1.155E-03	1.15475	0.45497	0.1439
396	0.396	6.566E+00	6.566E-01	1.114E-03	1.11430	0.44126	0.1082
398	0.398	6.589E+00	6.589E-01	1.187E-03	1.18715	0.47249	0.1716
400	0.4	6.614E+00	6.614E-01				

Integration Using trapazoidal rule from 0.208 to 0.398

	$E(\Theta)$	$\Theta * E(\Theta)$
Value of n	95	95
b-a	0.1900	0.1900
f(.208)	0.0017	0.0007
f(.398)	1.1871	0.4725
Sum f(.21)-f(.396)	328.8818	89.6471
Integral	0.6590	0.1798
Tail	0.3410	0.2337
Total	1.0000	0.4135

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Teaching Non-Ideal Reactors with CFD Tools

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Abstract

In this paper, a computational fluid dynamics (CFD) code (Fluent) was used to illustrate important concepts regarding residence time distribution (RTD) theory. The case study adopted considers isothermal laminar flow through 2-D reservoirs of different geometries (various length/height, L/H , ratios), and a tracer step input is simulated for RTD determination. From the steady-state solution, quasi-stagnant zones are easily identified, particularly for high flow rates (or, more rigorously, high Reynolds numbers) and for low L/H ratios. In some cases, the fraction of dead volumes amounts to values as high as 70%. For high L/H ratios one approaches the theoretical RTD for laminar flow between parallel plates. Transient simulations are also very useful because they allow ‘visualization’ of the evolution of tracer concentration fronts, which animation is available in our web site. The RTD obtained allows students to predict reactor’s performance, either in steady-state or transient regime. Such information can also be obtained directly from Fluent by simulating the injection of a reactive feed stream. The use of a commercially available CFD tool is illustrated to be advantageous, as it allows students to easily ‘visualize’ and understand the involved concepts, namely flow pattern and behavior/diagnosis of non-ideal reactors.

Keywords: RTD, CFD, Fluent, non-ideal reactors.

Introduction

Behavior of non-ideal reactors and their flow pattern characterization are issues taught in the majority of chemical reaction engineering (CRE) courses [1-4] (usually at undergraduate level, but this depends on the structure of the ChE curriculum), and therefore addressed in most CRE textbooks [*e.g.*, 5-8]. In this respect, the classical stimulus-response tracer experiments [9] are essential to obtain theoretical functions like the residence time distribution (RTD), which are crucial for diagnosis of equipment operation, reactor modeling and prediction of conversion. Comprehension of the involved concepts, which are not easily grasped by students, can be improved with laboratory sessions, but this is not always feasible. However, this disadvantage can be overcome by implementing computer simulation of tracer experiments [10], particularly with a commercial computational fluid dynamics (CFD) tool [11-13].

CFD codes have been widely used for simulating flow pattern in real systems and its use in a chemical engineering undergraduate course has several advantages, as mentioned by Sinclair [14]. Among them, we can mention the following: first, the use of color in CFD plots allows students to visualize the flow behavior, and this visualization of the flow phenomenon can significantly facilitate and enhance the learning process. Secondly, students can explore the effects of change in system geometry, system properties or operating conditions. All these advantages, apart from the fact that students like to experience software tools used in industry, which are usually user-friendly, justifies implementation of CFD codes in CRE courses, particularly when teaching RTD theory.

However, such tools also have some disadvantages and/or limitations. Codes commercially available may be extremely powerful, but their operation still requires a high level of skill and understanding from the operator to obtain meaningful results. In addition, CFD cannot be adequately used without continued reference to experimental and/or analytical validation of numerical results [13].

The case study described here can be implemented, for instance, as homework for students taking a CRE course dealing with non-ideal reactors. Simulations can be performed using a commercial package such as Fluent, but it is advisable that a brief tutorial is provided so that students can quickly familiarize with the program. In this tutorial, the essential steps that must be followed for any simulation should be outlined. Different reservoir/reactor geometries can be provided for different groups of two to three students, but each one should perform its own parametric study (*e.g.*, evaluate the effect of space-time, or Reynolds number, in flow pattern characterization, or Damköhler number in reaction simulations). They should finally compile the results obtained by other colleagues and discuss it in the final written report.

Using 2-D reservoirs/reactors with laminar flow, described in detail in the next section, students should perform the following tasks, which are also the objectives of the present paper: (i) characterize the hydrodynamics in the vessel(s); (ii) determine the RTD from tracer experiments, which includes diagnosis of reservoir/reactor operation; and (iii) predict the conversion in the continuous-flow system.

Case Study Formulation and Simulation with Fluent

It is well known that the mean residence time (\bar{t}_r) has an important effect in the performance of some large natural conversion systems such as biological lagoons, as it affects the biological conversion of biodegradable matter. Moreover, the geometry of the reservoirs seems to affect the RTD, and thus \bar{t}_r . It is therefore very important to perform tracer experiments in these systems (or try to estimate the RTD function) in order to better design such wastewater treatment plants. However, the mean residence times in these large reservoirs or lagoons are extremely high (ranging from one day up to several months [15,16]), so that tracer experiments are impracticable. Possible strategies to overcome this problem are: i) obtain the RTD on pilot-scale set-ups with various geometries, where tracer experiments are easily

conducted, and perform a scale-up analysis, and (ii) derive the RTD by solving the Navier-Stokes and diffusion-convection equations which students learned in fluid mechanics curricula [e.g., 16]. Commercially available CFD packages (e.g., Fluent, CFX, Fidap, Phoenix, STAR-CD, FLOW3D, etc.) can readily solve the balance equations for reactor operation coupled with the Navier-Stokes equations, and thus the second approach was herein adopted.

The case study presented considers a 2-D reservoir with dimensions L (length) and H (height), in laminar flow and isothermal conditions (see Figure 1). Reservoirs with different aspect ratios (L/H) were considered, varying between 0.5 and 20 (with $H = 0.1$ m). Both the inlet and the outlet boundaries of the reservoirs have a height of 0.01 m, which distances from the bottom of the reservoir are 0 and 0.02 m, respectively. A fully developed parabolic velocity profile is imposed at the inlet boundary:

$$u_x = U_{\max} \left[1 - \left(\frac{y - H/20}{H/20} \right)^2 \right] \quad (1)$$

where U_{\max} is the fluid velocity at the center of the inlet boundary, $U_{\max} = 1.5 U_{\text{mean}}$. A constant species concentration profile is assumed at the inlet boundary. On the walls (see Figure 1) no-slip conditions are assumed ($u_x = u_y = 0$) and a null flux (zero gradient) of species concentration is imposed. At the outflow boundary condition, the CFD code extrapolates the required information from the interior cells (a zero diffusion flux is assumed for all flow variables in the direction normal to the exit plane). In the simulations, the Reynolds number, here defined based on inlet conditions, was ranged from 1 to 100. Changing Re , for a given fluid and reservoir, is equivalent to change the fluid velocity (and thus the residence-time).

The governing equations to be solved are the following (for an incompressible fluid): continuity (Eq. 2), momentum (Eqs. 3 and 4) and the species transport equation (Eq. 5).

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0 \quad (2)$$

$$\rho \frac{\partial u_x}{\partial t} + \rho \left[\frac{\partial(u_x^2)}{\partial x} + \frac{\partial(u_x u_y)}{\partial y} \right] = -\frac{\partial P}{\partial x} + \mu \left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} \right) \quad (3)$$

$$\rho \frac{\partial u_y}{\partial t} + \rho \left[\frac{\partial(u_x u_y)}{\partial x} + \frac{\partial(u_y^2)}{\partial y} \right] = -\frac{\partial P}{\partial y} + \mu \left(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} \right) \quad (4)$$

$$\frac{\partial C}{\partial t} + \frac{\partial(u_x C)}{\partial x} + \frac{\partial(u_y C)}{\partial y} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) + S(C) \quad (5)$$

In Eq. (5) $S(C)$ is a source term. For the transport of an inert tracer, by convection-diffusion, $S(C) = 0$, while for the transport of a reagent species, $S(C) = -kC$ (assuming a 1st order irreversible reaction).

Simulations were run with the commercial package Fluent 6.0, from Fluent Inc.. The fluid considered is water ($\nu = \mu / \rho = 10^{-6} \text{ m}^2 \text{ s}^{-1}$), and a tracer solution was created in Fluent's database with identical properties of water, so that it does not affects reactor hydrodynamics. A molecular diffusivity of $5 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$ was considered, which is a typical value for liquids [17]. A tracer step input was used, with uniform concentration across the entrance section, together with the parabolic velocity profile defined in Eq. (1).

Fluent can simulate both the hydrodynamics and chemical reaction processes, and therefore the reservoirs previously considered can be used for modeling continuous-flow reactors (*e.g.* biological lagoons). In this case, simulations were run by defining a reactant and a product, both with properties identical to water. The reactor is initially full of water (inert), the laminar flow is established and after that, time $t = 0$, the reactant is fed to the reactor, similarly to the tracer step input. Conversion of reactant is calculated based on the time evolution of species concentration at the reactor exit, obtained from a mass-weighted average formulation.

We must point out that to achieve a high level of accuracy, all the simulation results presented in this paper involved a detailed analysis of the numerical algorithms, the mesh employed and the time step adopted (in transient simulations). For instance, the QUICK scheme of Leonard [18] was selected for discretisation of the convective terms, a 2nd-order implicit

formulation was used during unsteady simulation and the computational grid contained typically 100×100 elements (note that for reservoirs with $L/H \gg 1$, it is convenient to use a larger number of cells in the x -direction). It is always a good practice to perform the calculations on several meshes with different levels of refinement, in order to obtain mesh-independent results. A similar procedure should be adopted regarding the time step used in transient calculations. A control-volume approach is used by Fluent to numerically solve the governing equations [11].

Results and Discussion

i) Hydrodynamic characterization

Figure 2 shows a contour plot of the stream function within the reservoir with $L/H = 1$, which illustrates the trajectories of the fluid elements (streamlines). For a given inlet velocity, or more broadly speaking a given Reynolds number, it is evident the formation of a recirculation zone above the entrance of the reservoir, where velocity is small, thus suggesting formation of a stagnant region. It is noteworthy that the importance of such region increases with Re , becoming particularly large for Re values around 100 where fluid trajectories are almost linear. Lower Reynolds numbers leads to a smaller stagnant region and more curved streamlines. For $Re < 1$ the inertia is negligible, and the trajectories obtained are equivalent to creeping flow conditions.

For longer reservoirs the conclusions are similar, but now the importance of the recirculation zone decreases (for the same fluid inlet velocity). Indeed, the steady state streamlines shown in Figure 3, obtained for a reservoir with $L/H = 5$, show the formation of a stagnant zone above the entrance, which size increases with the Reynolds number. However, comparison with the stream function contours of Figure 2 shows that for the same Re , the fraction of dead volume decreases when the geometric ratio L/H increases.

ii) RTD determination from tracer experiments

After performing steady state simulations, students may proceed to transient runs. However, they must first define a tracer step input at the inlet boundary condition. They must also be aware that for $t = 0$ no tracer exists within the reservoir and that the laminar flow is already established. So, they must first initialize the entire domain with a null tracer concentration, and wait until the laminar regime is established before introducing the tracer step change at inlet. After that, the CFD code solves the convection-diffusion equation that describes the tracer transport in the reservoir, and one obtains the concentration field of tracer under transient regime. Particularly interesting is its concentration at the outflow boundary, $C_{out}(t)$. The contours of tracer concentration throughout the reservoir along time are also very interesting because they provide a good perspective on the evolution of concentration fronts. For the reservoir with $L/H = 1$, some frames were recorded at different times, which are shown in Figure 4. They show that only for $\theta = t/\tau$ around 0.22 one start to ‘see’ tracer at the reservoir exit. In addition, even for a very long time of operation (about 5 times the residence time), the reservoir is not completely full of tracer, due to the stagnant zone previously identified. To better illustrate this transient behavior, it is possible to create an animation sequence with Fluent, using several frames obtained from the previous simulation. This was done and is available in the website: <http://www.fe.up.pt/~mmalves/cfd/reactor/index.htm>.

With the data of transient tracer concentration at the outlet of the reservoir, which can be exported to an ASCII file, students can then compute the so-called Danckwerts’ F curve, the normalized response of the reactor to a step input:

$$F(t) = \frac{C_{out}(t)}{C_{in}} \quad (6)$$

Data can then be manipulated with a spreadsheet program, such as Microsoft ExcelTM. Results shown in Figure 5 evidence the expected F curve, which only reaches the asymptotic value of 1 for very long times. It is worth mentioning the use of a logarithmic time scale, showing that

tracer starts to exit the reservoir at around $\theta = t/\tau = 0.22$ due to its transport by convection, while fluid elements that enter the stagnant region only come out, by diffusion, much later (see detail of Figure 5).

With the response to a step input, the RTD function can now be computed:

$$E(t) = \frac{dF(t)}{dt} \quad (7)$$

or, in terms of reduced time θ :

$$E(\theta) = \frac{dF(\theta)}{d\theta} = \tau \cdot E(t) \quad (8)$$

Figure 6 shows the RTD curves as a function of the Reynolds number, which gives an idea, for a given fluid, how space-time affects the RTD function. In all cases, the RTD curves evidence a very long tail and that a large fraction of fluid elements exits the reservoir with ages younger than the space-time, τ . Both features are indicative of the existence of large stagnant regions, together with slow recirculating flows near the inlet, as shown in Figure 2. It is also visible from Figure 6 that Re affects the RTD curve. Higher Reynolds numbers imply that the fluid elements start to leave the reactor sooner and a higher fraction of fluid elements has a smaller residence time.

The effect of the reservoir geometry on the RTD is shown in Figure 7. It can be seen that when L/H increases the curves are shifted to the right, *i.e.*, the mean residence time seems to increase because the importance of the recirculating zone decreases. This was previously found in the steady-state streamlines shown in Figures 2 and 3. It is particularly noteworthy that for very long reservoirs one tends towards an asymptotic $E(\theta)$ curve, also shown in Figure 7. This curve corresponds to the case of laminar flow between parallel plates, given by [19]:

$$E(\theta) = \begin{cases} \frac{1}{3\theta^3 \sqrt{1 - \frac{2}{3\theta}}} & \theta \geq \frac{2}{3} \\ 0 & \theta < \frac{2}{3} \end{cases} \quad (9)$$

It must be stressed that for this situation, *i.e.*, laminar flow between parallel plates, the parabolic profile is characterized by a maximum velocity, at the center, which is 1.5 times the average velocity, while for flow in pipes this ratio is 2.

The RTD functions can then be used to calculate the mean residence time, defined as:

$$\bar{t}_r = \int_0^{\infty} t \cdot E(t) dt \quad (10)$$

or,

$$\bar{\theta}_r = \frac{\bar{t}_r}{\tau} = \int_0^{\infty} \theta \cdot E(\theta) d\theta \quad (11)$$

For a closed-closed system (*i.e.*, with no dispersion), and if no bypass or stagnant regions exists, it is well known that the mean residence time and space-time are equal [7,20]. However, due to the very long tail of the RTD function, this is only verified if simulations are run up to very high times (typically θ of $O(10^3)$). Otherwise, the normalization condition $\int_0^{\infty} E(t) dt = \int_0^{\infty} E(\theta) d\theta = 1$ is not satisfied, and the computed mean residence time is smaller than the real space-time.

Calculation of the mean residence time is very important for evaluation of malfunctions during reactor's operation. Indeed, a straightforward way to diagnose the reactor's flow performance consists in comparing the computed value of the mean residence time from Eq. (10) with the space-time ($\tau = V / Q$, where V is the total volume of reactor and Q the volumetric flow rate), which is equivalent to compare $\bar{\theta}_r$ with 1. Disagreement between these two values may indicate the existence of bypasses, dead volumes, etc. For instance, as indicated by Froment [5], if a region of the vessel retains a portion of the fluid for an order of magnitude greater than the

mean residence time of the total fluid, then, for all practical purposes, that portion is essentially at rest and the region is wasted space in the vessel.

The values obtained for the mean residence time shown in Tables 1 and 2 were calculated by integration of the RTD curves up to $\theta = 10$. It is evident that they strongly dependent on both the Reynolds number and the geometry of the reservoir. As Re decreases, the mean residence time increases (Table 1). As expected, when L/H increases, the mean residence time approaches the space-time value (Table 2).

Because in all cases $\bar{t}_r < \tau$, or $\bar{\theta}_r < 1$, we can conclude that a stagnant region exists, which in practice would be a dead volume, leading to a lower reactor performance. The fraction of the reactor volume occupied by the dead region is given by [6,20]:

$$\frac{V_d}{V} = 1 - \frac{\bar{t}_r}{\tau} \quad (12)$$

The dead volume fractions obtained, shown in Tables 1 and 2, indicate that for high Re values (or high fluid velocities) and for geometries where L/H approaches 1, or even smaller, a large fraction of the reservoir will not be efficiently used for reaction purposes.

iii) Prediction of conversion in the continuous-flow reactor

In a real reactor, the RTD function can be used to predict the limiting values of conversion under the two extremes of micromixing, using the well known total segregation or maximum mixedness models [21]. However, for first-order reactions (linear systems), the state of mixing does not affect conversion [20], and therefore the easy-to-use segregation approach can be applied to predict reactor performance. The total segregation model assumes that all fluid elements having the same age (residence time) “travel together” in the reactor and do not mix with elements of different ages, until they exit the reactor [7]. Because there is no interchange of matter between fluid elements, each one acts as a batch reactor and so the mean steady-state conversion (\bar{X}) in the real reactor is given by:

$$\overline{X} = \int_0^{\infty} X_{batch}(t) \cdot E(t) dt = \int_0^{\infty} X_{batch}(\theta) \cdot E(\theta) d\theta \quad (13)$$

where $X_{batch}(t)$, for a first-order reaction, is given by:

$$X_{batch} = 1 - e^{(-k \cdot t)} = 1 - e^{(-Da \cdot \theta)} \quad (14)$$

and $Da = k\tau$ is the Damköhler number.

Steady-state conversion is then computed by students using Eq. (13), with the RTD function previously determined. It is important to remark that the segregation model can also be used for prediction of the reactor transient behavior. In this case, the upper integration limit in Eq. (13) must be set to t (or θ). This was done for our case study and the results shown in Figure 8 illustrate the reactant conversion in transient conditions, up to steady state, for different Damköhler values. One must take care that the RTD used for prediction of reactor performance depends on its geometry and on the Reynolds number. In addition, because of the very long tail of the RTD function (as shown in Figure 5 for the $F(\theta)$ curve), prediction of steady-state conversion requires RTD data up to very large times (note the logarithmic time scale). This interesting feature is also evident in Figure 8: a non-negligible contribution to the overall reactor performance (in terms of fractional conversion), which is noticed at very long times. Such behavior can be attributed to the stagnant region and to the different time scales for the involved phenomena: reaction, convection and molecular diffusion.

As mentioned above, Fluent can also be used to simulate the system in the presence of a reaction, and so the data shown in Figure 8 can be obtained either through the total segregation model, or directly from CFD simulations (obtained curves coincide). Asking students to compare results from both approaches is important because they feel more confident about the simulation results and calculations.

Simulation of the continuous-flow reactor via CFD can also be used to evidence the contours of species concentration throughout the reactor, for instance at steady-state. Such nice

color pictures can also be seen in our web site: <http://www.fe.up.pt/~mmalves/cfd/reactor/index.htm>. The color gradient inside the reactor is particularly interesting to observe.

Finally, it is convenient to ask students to compare the steady-state conversion attained in the real reactor with those achieved with the ideal reactors that they learned in previous CRE courses: continuous stirred tank and plug flow reactors. For a first-order reaction, performance achieved by these reactors is given by [e.g., 7,8]:

$$X_{CSTR} = \frac{Da}{1 + Da} \quad (15)$$

$$X_{PFR} = 1 - e^{(-Da)} \quad (16)$$

Data shown in Figure 9 indicate that when dead regions or stagnant zones are negligible, *i.e.* for geometries where L/H is higher than about 5 (for $Re = 10$), the performance of the real reactor lies between that of the CSTR and PFR. When L/H is close to 1, or even smaller, such anomaly (dead volume) leads to a much lower performance of the non-ideal reactor, even lower than that achieved with a perfectly mixed reactor. It is also noteworthy that for very long reactors (*i.e.* high L/H ratios), one approaches the theoretical behavior of a laminar flow reactor (flow between parallel plates), computed using the RTD function given in Eq. (9) and the segregation model.

Concluding Remarks

Concepts dealing with the RTD theory and non-ideal reactors are not very familiar to undergraduate students, and thus it is not an easy task to teach these matters in CRE courses. Explanation of how stimulus-response tracer experiments provide the theoretical functions which are crucial for reactor's diagnosis, prediction of conversion, etc., becomes clearer through experimentation, which is not always feasible. For such purpose, the use of CFD packages has

been particularly advantageous. Besides, CFD tools provide a graphical portrait of flow throughout the reservoir/reactor, thus allowing going beyond simply predicting what will come out of the reactor to predicting all of the properties of interest within the reactor. Some of the concepts involved are more easily understood, like the progression of the tracer concentration front, the formation of dead volumes or the existence of a concentration profile along the reactor. Therefore, implementation of a CFD code has a considerable pedagogical content.

The case study herein described, a 2-D lagoon with laminar flow, was solved with the commercial package Fluent. Using reservoirs/reactors with different geometries and/or different operating conditions, students are asked to: (i) characterize the hydrodynamics; (ii) determine the residence time distribution from tracer experiment, which provides diagnosis of reactor operation; and (iii) predict conversion in a continuous-flow reactor (both steady-state and transient behavior). Our experience shows that the use of the CFD code allows students to more easily understand some of the basic concepts taught in CRE curricula. Finally, comparison of numerical with analytical solutions known for laminar flow between parallel plates (*i.e.*, for geometries with high L/H ratios), improves their self-reliance regarding CFD results.

In a survey performed a few years ago to several chemical engineering departments spread all over the world, some of the main points addressed by the departments to a question relating to the future of CRE courses were [2]: i) the increasing importance of computer applications and software packages and ii) put more emphasis on non-ideal reactors. With the case study herein proposed, both issues are dealt with, therefore meeting current trends in CRE instruction. In addition, students face the potential of CFD codes, which have been successfully used in practice to design commercial-size reactors, usually with complex flow processes [22].

Nomenclature

C = concentration of tracer, reactant or product (mol.m^{-3} or kg.m^{-3});

D = coefficient of diffusivity ($\text{m}^2.\text{s}$);

Da = Damköhler number, dimensionless;

$E(t)$ = residence-time distribution function (s^{-1});

$E(\theta)$ = normalized RTD function, dimensionless;

$F(t)$ = Danckwerts' F curve, dimensionless;

H = height of the reservoir/reactor (m);

k = reaction rate constant of the first-order reaction (s^{-1});

L = length of the reservoir/reactor (m);

P = pressure (Pa);

S = source term ($\text{mol m}^{-3} \text{s}^{-1}$ or $\text{kg m}^{-3} \text{s}^{-1}$);

Q = volumetric flow rate ($\text{m}^3 \text{s}^{-1}$);

Re = Reynolds number, dimensionless;

t = time (s);

\bar{t}_r = mean residence time (s);

U_{max} = fluid velocity at the center of the inlet boundary (m.s^{-1});

U_{mean} = mean fluid velocity at the inlet boundary (m.s^{-1});

u_x = x-velocity (m.s^{-1});

u_y = y-velocity (m.s^{-1});

V = volume of reservoir/reactor (m^3);

V_d = dead volume in the reservoir/reactor (m^3);

X = conversion, dimensionless;

x = horizontal co-ordinate (m);

y = vertical co-ordinate (m);

Subscripts

batch = refers to batch reactor;

CSTR = continuous stirred tank reactor;

in = inlet conditions;

PFR = plug flow reactor;

out = outflow conditions;

Greek Symbols

$\theta = t/\tau$ = reduced time, dimensionless;

$\bar{\theta}_r = \bar{t}_r / \tau$ = reduced mean residence time, dimensionless;

μ = viscosity of the fluid ($\text{kg m}^{-1}\text{s}^{-1}$);

ν = kinematic viscosity of the fluid (m^2s^{-1});

ρ = density of the fluid (kg m^{-3});

τ = space-time (s);

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TABLE 1

Influence of the Reynolds Number in the Mean Residence Time and Fraction of Dead Volume (reservoir with $L/H = 1$). Values Calculated from RTD Curves up to $\theta = 10$.

Re	Mean Residence Time	Fraction of Dead Volume
	$\overline{\theta_r} = \frac{\overline{t_r}}{\tau}$	$\frac{V_d}{V}$
1	0.778	0.222
5	0.724	0.276
10	0.412	0.588
20	0.318	0.682
100	0.261	0.739

TABLE 2

Influence of the Reservoir Geometry in the Mean Residence Time and Fraction of Dead Volume (for $Re = 10$). Values Calculated from RTD Curves up to $\theta = 10$.

L/H	Mean Residence Time	Fraction of Dead Volume
	$\overline{\theta_r} = \frac{\overline{t_r}}{\tau}$	$\frac{V_d}{V}$
0.5	0.300	0.700
1	0.412	0.588
2	0.752	0.248
5	0.935	0.065
10	0.992	0.008
20	0.997	0.003

Figure Captions

Figure 1: Sketch of reservoir geometry.

Figure 2: Steady state contours of the stream function for the reservoir with $L/H = 1$ as a function of the Reynolds number.

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Figure 4: Transient tracer concentration contours for the reservoir with $L/H = 1$ ($Re = 10$).

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Figure 8: Unsteady-state conversion obtained for the reactor with $L/H = 1$, predicted from the segregation model ($Re = 10$).

Figure 9: Steady-state conversion versus Damköhler number for reactors with different geometries ($Re = 10$).

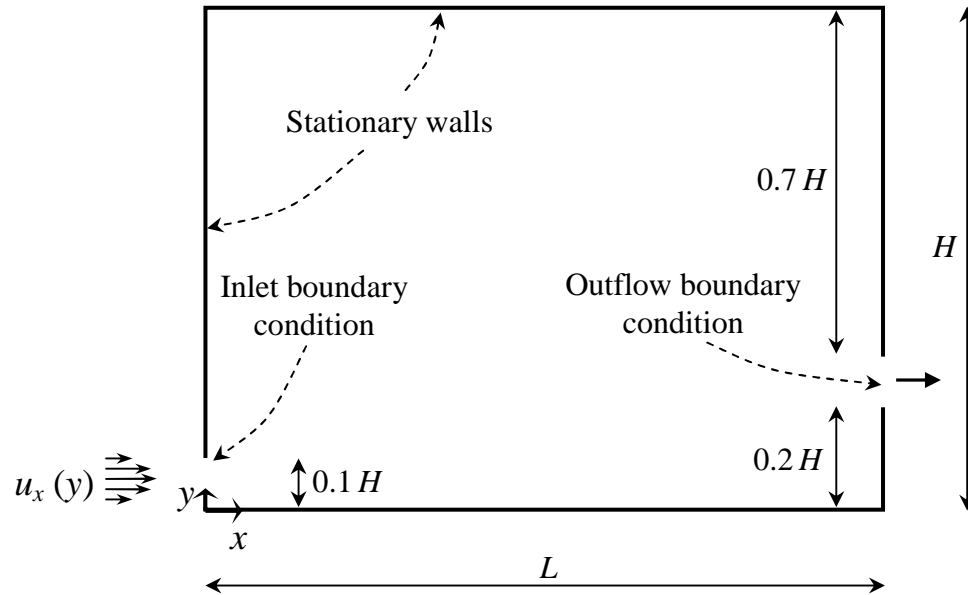
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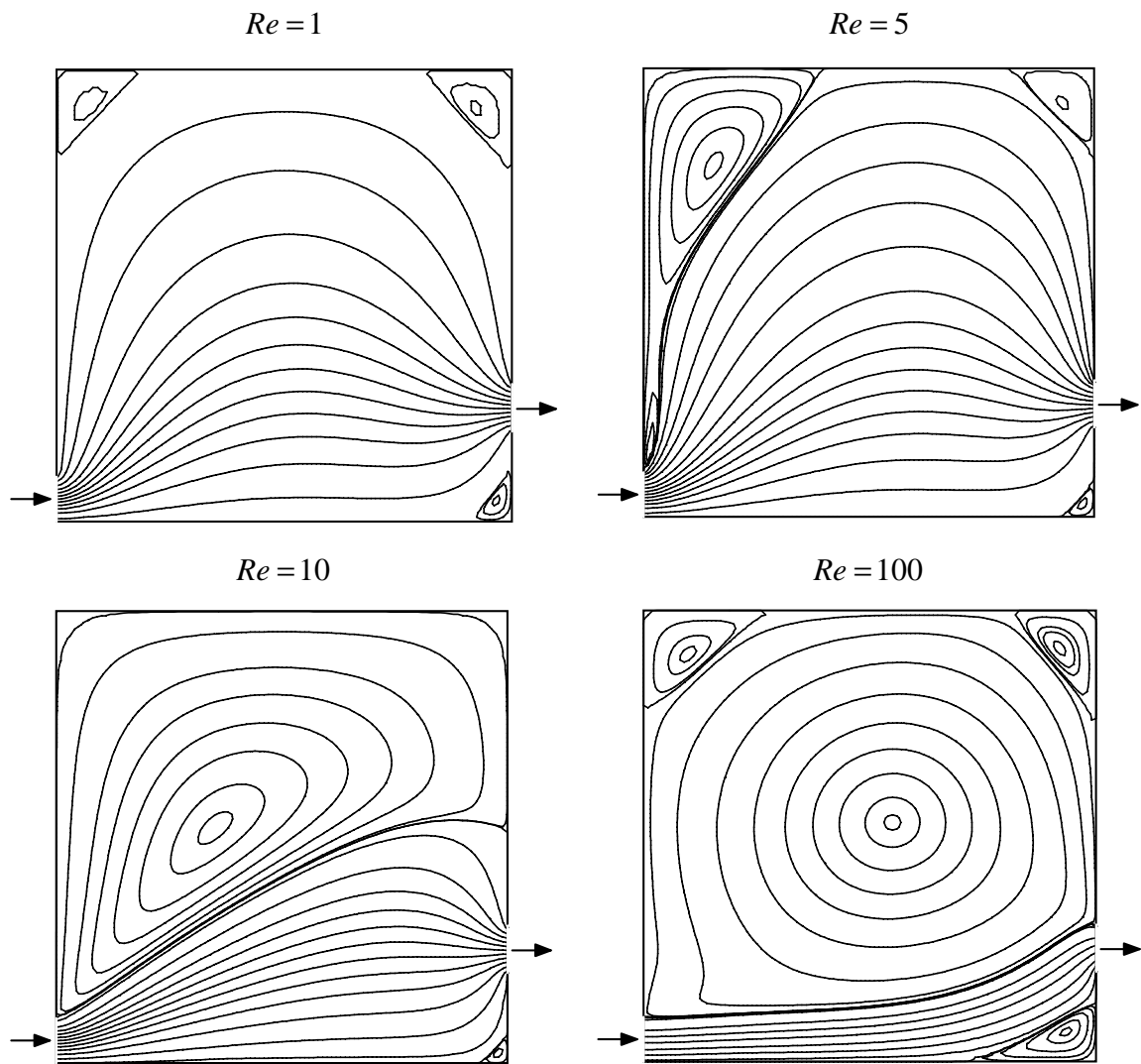
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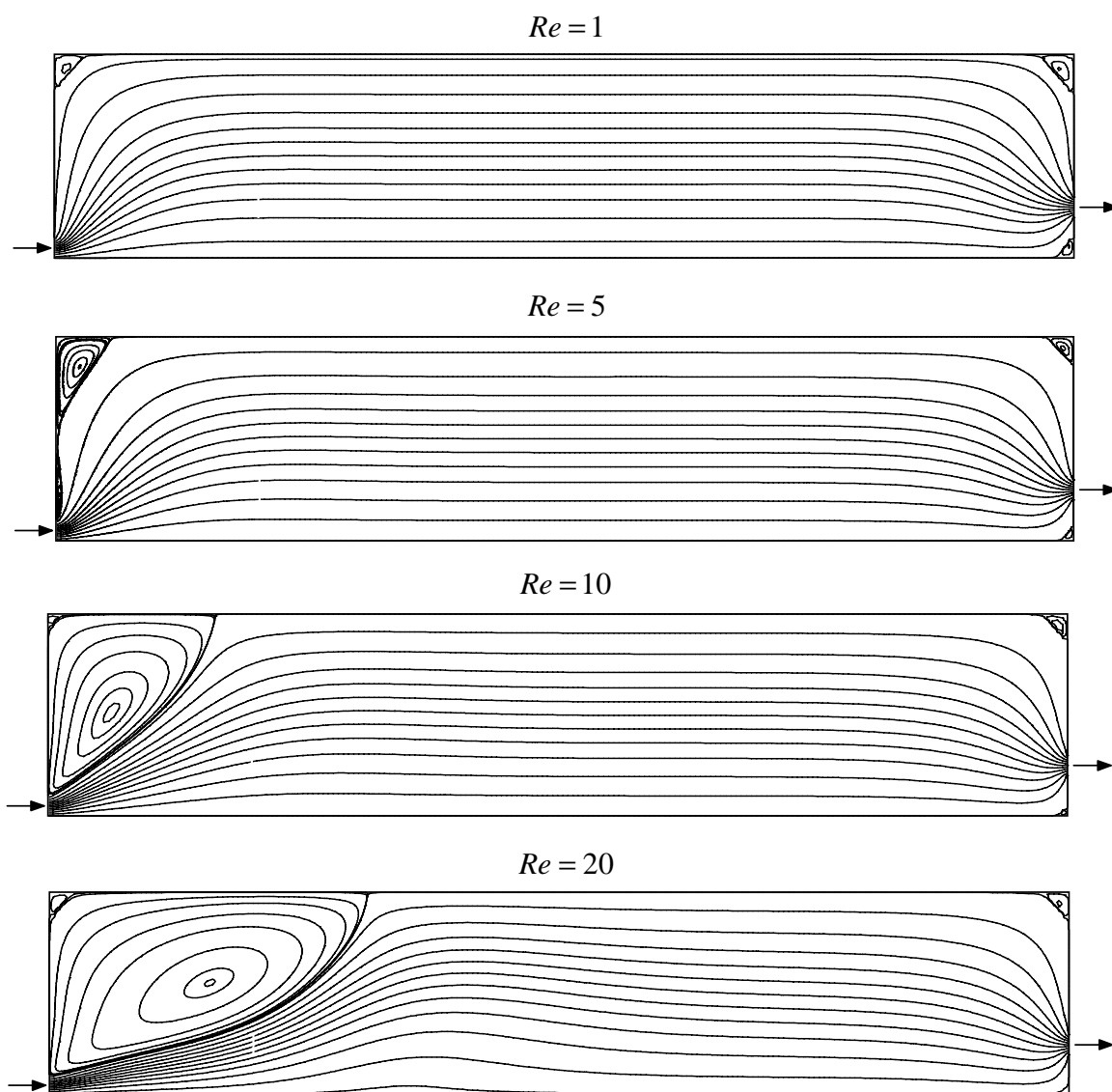


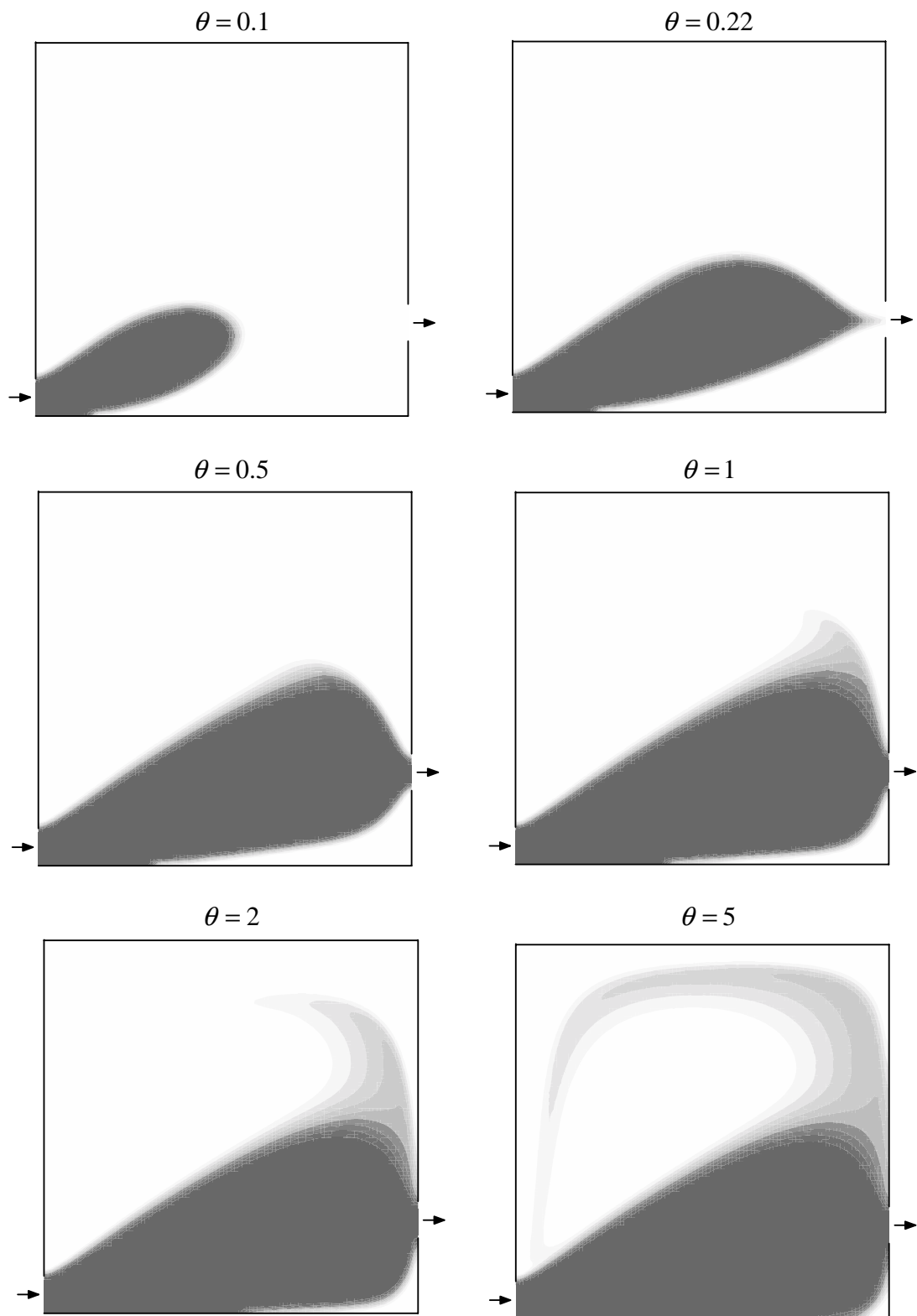
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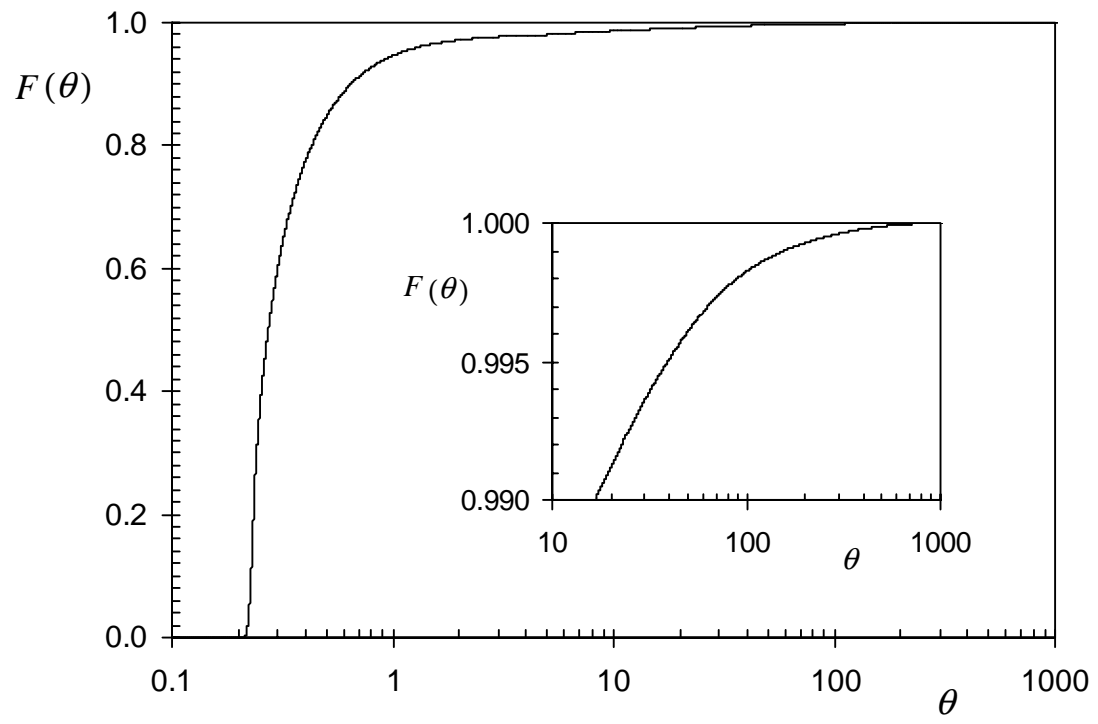
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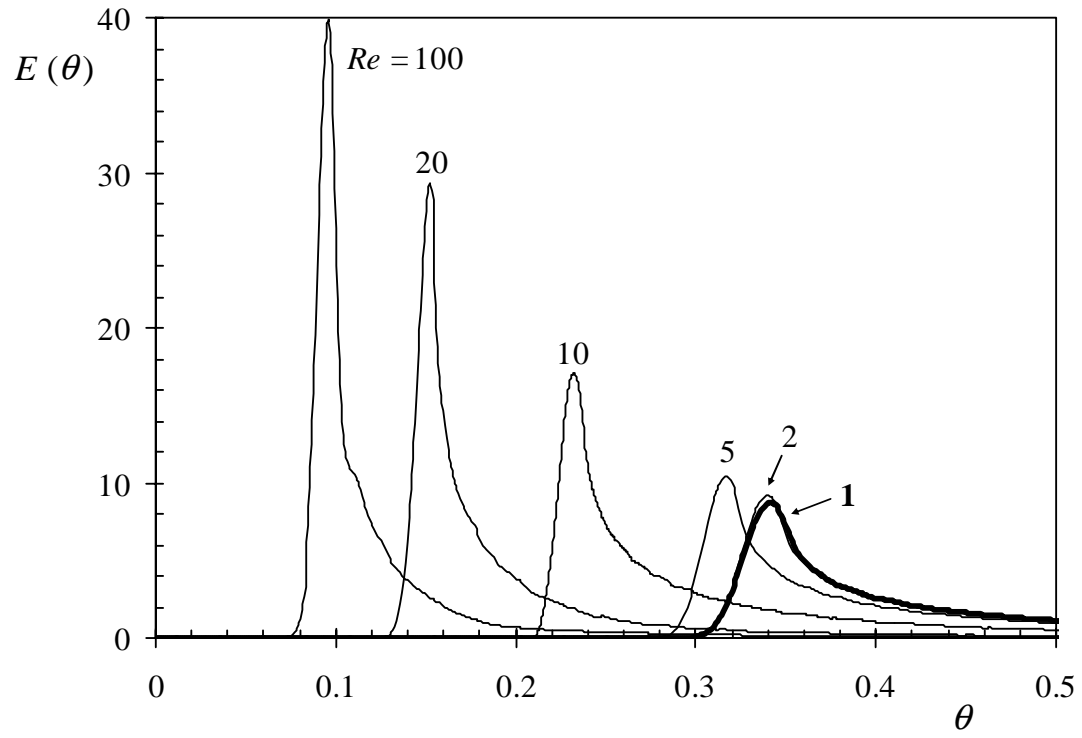
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Figure 7

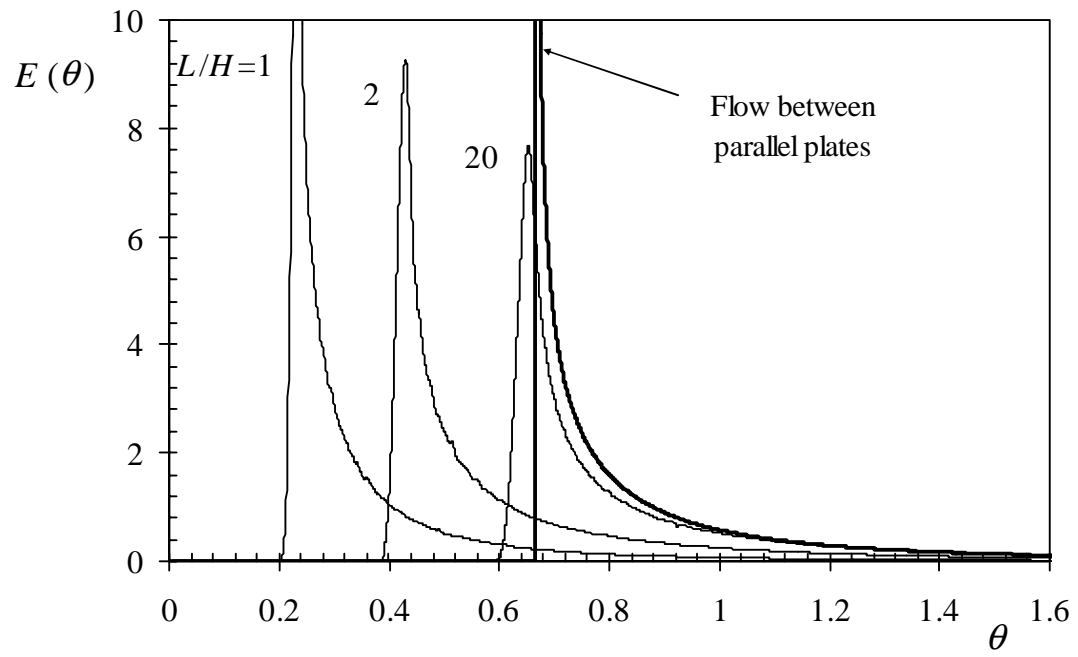


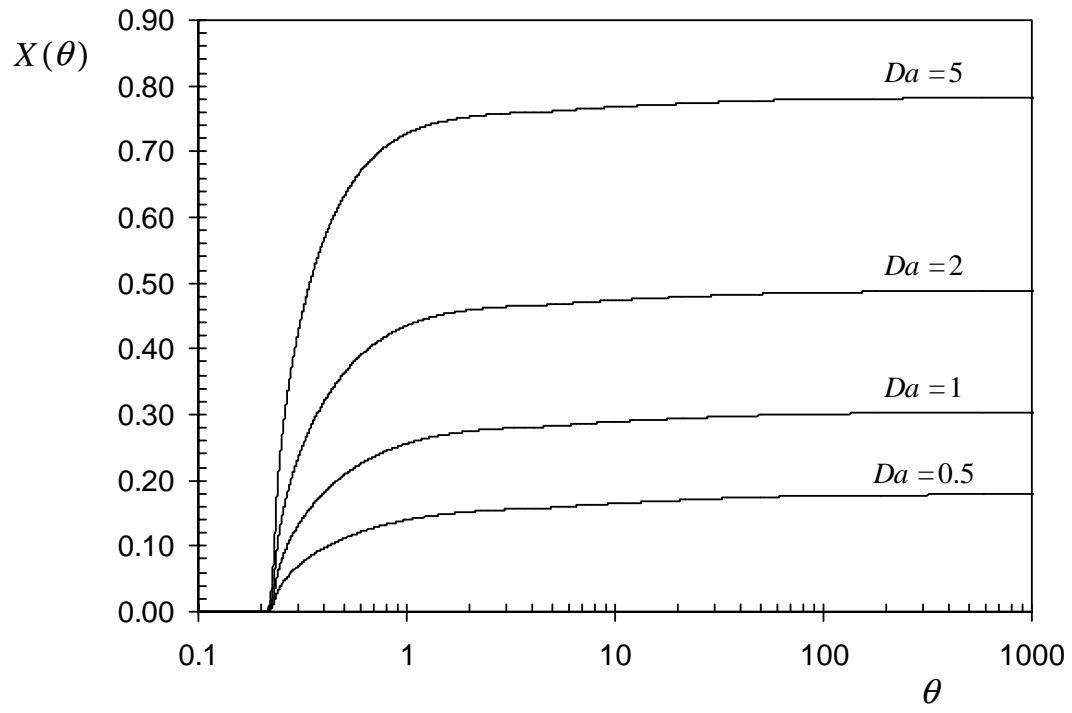
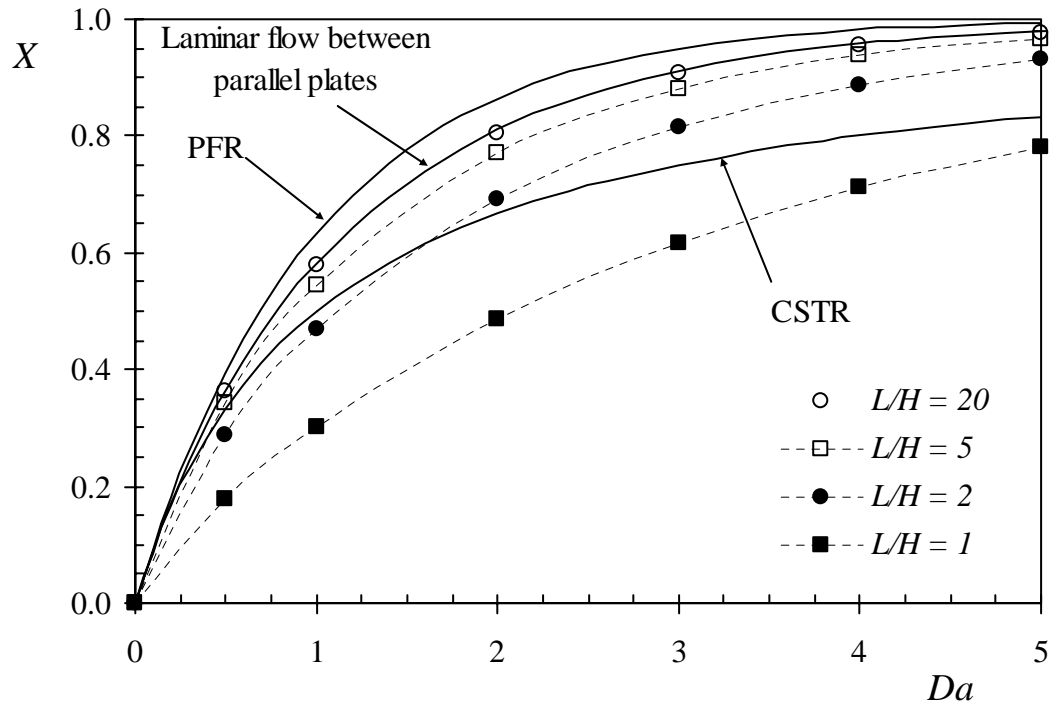
Figure 8

Figure 9





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Development of *Hands-On* CFD Educational Interface for Undergraduate Engineering Courses and Laboratories

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Abstract

Development described of an educational interface for *hands-on* student experience with computational fluid dynamics (CFD) for undergraduate engineering courses and laboratories. Project part of a three-year National Science Foundation sponsored Course, Curriculum and Laboratory Improvement - Educational Materials Development project with faculty partners from colleges of engineering at Iowa, Iowa State, Cornell and Howard universities along with industrial (commercial CFD code) partner FLUENT Inc, including complementary experimental fluid dynamics and uncertainty analysis. The design of the educational interface teaches students CFD methodology (modeling and numerical methods) and procedures through interactive implementation that automates the CFD process following a step-by-step approach. The CFD process mirrors actual engineering practice: geometry, physics, mesh, solve, reports, and post processing. Predefined active options for students' exercises use a hierarchical system both for introductory and advanced levels and encourages individual investigation and learning. Ideally, transition for students would be easy from advanced level to using FLUENT or other industrial CFD code directly. Generalizations of CFD templates for pipe, nozzle, and airfoil flows facilitate their use at different universities with different applications, conditions, and exercise notes. Implementation based on results from site testing at faculty partner universities for an introductory fluid mechanics course at Iowa, for aerodynamics and gas dynamics laboratory courses at Iowa State, for a required fluid mechanics sequence at Cornell, and for an aerodynamics course at Howard. The evaluation and research plan (created in collaboration with a third party program evaluation center at the University of Iowa) is described, which focuses on exact descriptions of the implementations of the new interface at partner sites, especially as experienced by the students, including preliminary data on immediate student outcomes as documented from site testing for Fall 2003. Also discussed are conclusions and future work.

Introduction

As simulation based design and ultimately virtual reality become increasingly important in engineering practice, it becomes equally important to integrate simulation technology into the undergraduate engineering curriculum. Simulation technology covers a broad range from computerized systems to computerized solutions of engineering problem formulations using mathematical physics modeling, numerical methods, and high performance computing; all of which broadly influences all engineering disciplines. Pedagogy of integration of simulation technology into the undergraduate engineering curriculum and pedagogy of computer-assisted learning are related. The latter includes web-based teaching, CDROM, robotics, studio arts, remote experiments, and computer-based textbooks. Of present interest is integration of computational fluid dynamics (CFD) into undergraduate engineering courses and laboratories. CFD is a widely used tool in fluids engineering with many specialty and commercial CFD codes through out the world covering many application areas. One major obstacle to the greater use of CFD is lack of trained users.

Fluid mechanics courses are included in the curricula of most engineering programs, with both program required and technical elective courses. Program required courses are at both the introductory and advanced levels, whereas technical elective courses are at advanced levels. More than one program often requires introductory level courses (e.g., mechanical, civil, and bio engineering departments) or combined with related subjects such as thermodynamics, heat transfer, and chemical and aerospace engineering. Most introductory courses are textbook based with emphasis on analytical fluid dynamics (AFD) and problem solving with or without experimental fluid dynamics (EFD). EFD used primarily to demonstrate physics with limited consideration of EFD methodology and uncertainty analysis (UA). CFD is seldom included. A notable exception is the multi-media classroom developed at Worcester Polytechnic University for demonstrating relationship between analytical, numerical, and experimental methods¹ and the work of the authors², as described later. Advanced level courses are usually AFD with or without EFD and/or CFD assignment or EFD including methodology and in some cases UA. Recent developments have focused on development of CFD courses using specialty^{3,4} and commercial⁵⁻⁷ software, which are sometimes combined with EFD^{8,9}. Computer assisted learning has also impacted fluid dynamics courses, such as using multi-media in teaching fluid mechanics¹⁰, application of studio model¹¹, and development of computer-based textbook¹². These studies have shown enhancement of the curriculum, increased learning efficiency and understanding, effectiveness of novel and *hands-on* learning methods, importance and need for educational interface design and pedagogy, and positive student response.

Authors² have contributed to integration of simulation technology into undergraduate engineering courses and laboratories through collaboration on the development of teaching modules (TM) for complementary CFD, EFD, and UA, including lectures on CFD, EFD, and UA methodology and procedures; CFD templates for academic use of commercial CFD; and exercise notes for use of CFD templates and complementary EFD and UA. The commercial CFD code is FLUENT. TMs based on *proof of concept* developed at The University of Iowa. Project supported by National Science Foundation 3-year award for faculty partners from colleges of engineering at large public (Iowa and Iowa State) and private (Cornell) and

historically minority private (Howard) universities for collaboration on further development TMs, effective implementation, evaluation, dissemination, and pedagogy of simulation technology utilizing web-based techniques. The evaluation and research plan included collaboration among faculty and the University of Iowa, Center for Evaluation and Assessment. During the first year, pipe, nozzle, and airfoil TMs were successfully developed, implemented, and evaluated for an introductory fluid mechanics course at Iowa, for aerodynamics and gas-dynamics-laboratory courses at Iowa State, for a required fluid mechanics sequence at Cornell, and for an aerodynamics course at Howard. The evaluation results showed similar trends to other related studies and additionally used for formative evaluation purposes¹³, as a guide for further developments CFD templates: educational interface for *hands-on* teaching CFD process, facilitating site testing same CFD template at different universities with different exercise notes, and broader dissemination. Here, *hands-on* defined as the use of EFD, CFD, and UA engineering tools in meaningful learning experience, which mirrors as much as possible *real-life* engineering practice.

The present paper describes the second-year project effort specifically on development of CFD educational interface for pipe, nozzle, and airfoil flows, including design for teaching CFD methodology and procedures, implementation based on site testing at partner universities, and evaluation. The evaluation based on field-testing investigates student learning and benefit from the revised efforts. Also discussed are further developments of CFD lecture, conclusions, and future work.

CFD Educational Interface

Whether or not specialty or commercial software used for teaching CFD, an educational interface to facilitate students' learning is required. Commercial software has the advantage that students may likely use same or similar software as professionals. Ideally, using educational interface at advanced level is essentially same as using commercial software itself.

Proof of concept (1999-2002) used FLUENT directly, which required lengthy detailed instructions (setting many parameters that were often unrelated to student application and difficult to explain or connect to a general CFD process) and did not facilitate options for modeling, numerical methods, and verification and validation studies.

Initiation present project coincided FLUENT release Flowlab version 1.0 (2002). The design of Flowlab was as a general-purpose CFD template, enabling students to solve predefined exercises. During the first year of the project, faculty partners collaborated with FLUENT Inc. on setting up templates for their respective courses and/or laboratories with agreed focus on introductory level and pipe and airfoil exercises. Collaboration faculty partners and FLUENT focused on modifications of Flowlab operations menu to more accurately reflect CFD process and capability and accuracy for specific student applications, including comparisons with AFD or EFD validation data. The evaluation confirmed that the implementation was worthwhile and promising, but at same time indicated direction for improvements. (1) Use of different specialized CFD templates for each exercise implied different CFD process for each application and did not facilitate site testing. (2) Exercises lacked options and depth. (3) Overly automated.

(4) Non-user-friendly interface was difficult to use. (5) Performance accuracy and flow visualization were substandard. Student anonymous responses suggested that students agree EFD, CFD, and UA labs were helpful to their learning fluid mechanics and important *tools* that they may need as professional engineers; however, they would like that learning experience to be more *hands-on* and tailored to their learning needs. Collaboration faculty partners and FLUENT during the second year of the project focused on development, implementation, and evaluation of the *hands-on* CFD educational interface.

Design Specifications The CFD educational interface designed to teach students CFD methodology (modeling and numerical methods) and procedures through interactive implementation for engineering applications. The CFD process is automated following a step-by-step approach, which seamlessly leads students through setup and solution of initial boundary value problem for application at hand. The CFD process mirrors actual engineering practice: geometry (solid and other fluid boundaries), physics (fluid properties, modeling, initial and boundary conditions), mesh, solve (numerical parameters), reports (monitor solution convergence), and post processing (flow visualization, analysis, verification, validation using imported EFD data and uncertainties). Predefined active options for students' exercises use a hierarchical system both for introductory and advanced levels and encourages individual investigation and learning. Ideally, transition for students would be easy from advanced level to using FLUENT or other industrial CFD code directly. A dynamically updated sketch window monitoring progress and enabling input parameter specifications is planned for future developments in conjunction with extensions for advanced level CFD templates, as will be discussed later. Generalizations of CFD templates for pipe, nozzle, and airfoil flows facilitate their use at different universities with different applications, conditions, and exercise notes using Flowlab version 1.1 (2003).

Pipe and Nozzle Flow Fig. 1 is a screen dump of the pipe flow template at a specific step of the CFD process and a flow chart for the pipe flow template showing all current active options available for students. Fewer active-options are available to students for the pipe flow than the airfoil flow template. The nozzle template is similar.

Airfoil Flow Fig. 2 is a flow chart for the airfoil flow CFD template showing all current active options available for students. More active-options are available to students for the airfoil flow than the pipe flow CFD template.

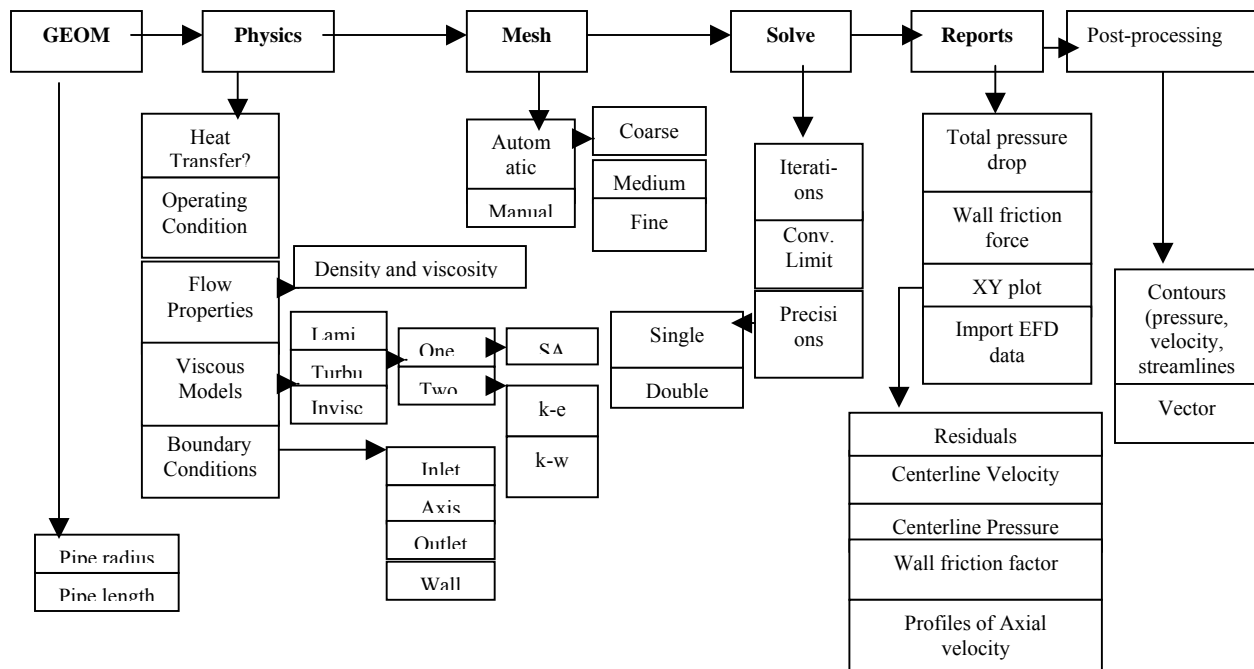
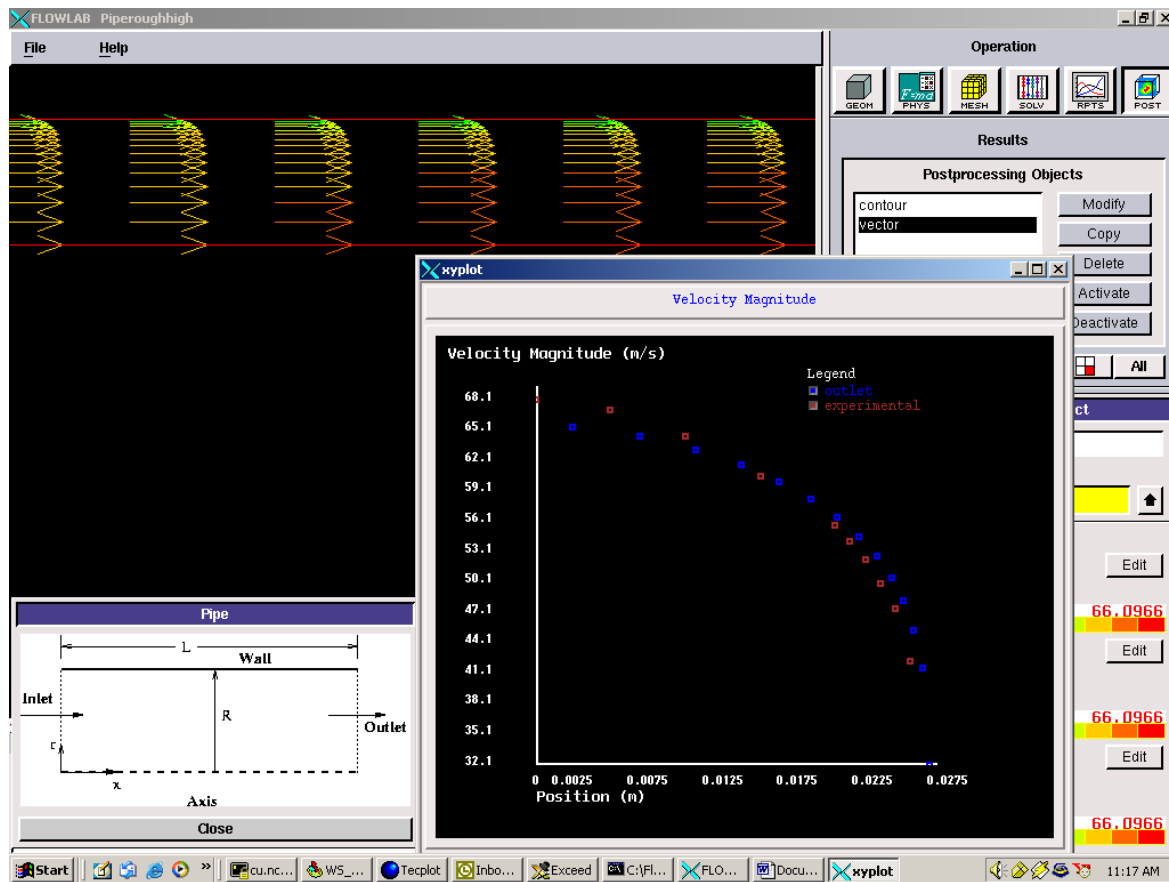


Fig. 1 Screen dump and flow chart for the pipe flow CFD template.

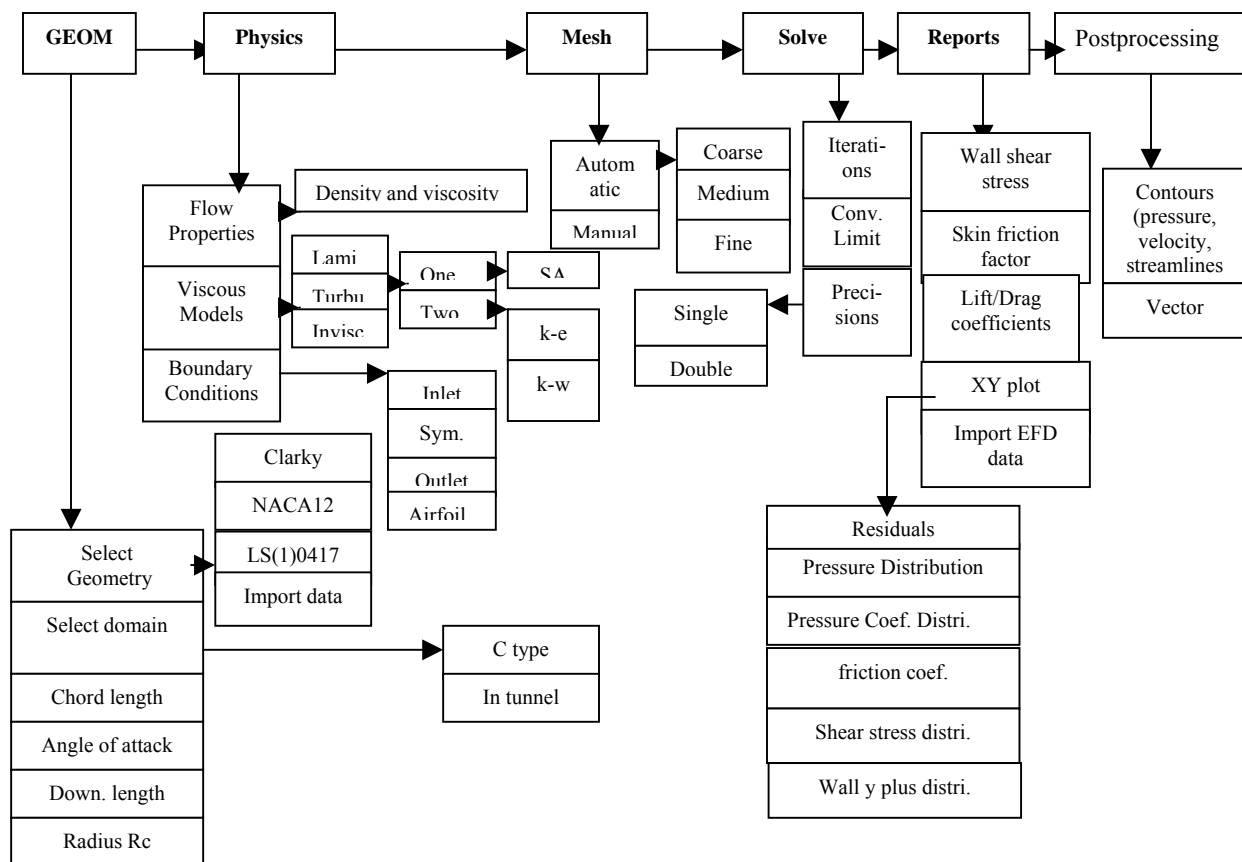


Fig. 2. Flow chart for the airfoil flow CFD template.

CFD Lecture Purpose of the CFD lecture is to prepare students for use of CFD educational interface using only one or two classroom 50-minute lectures. In general, faculty agreed on need, content (what, why, and where CFD; modeling; numerical methods; types of CFD codes; CFD process; example; and CFD educational interface and student applications), and desirability of collaboration on development of a common CFD lecture that could be site tested at different universities similarly as CFD educational interface. However, presently CFD lectures are not combined such that status described next in conjunction with site testing.

Site Testing

Site testing conducted for an introductory fluid mechanics course at Iowa, for aerodynamics and gas-dynamics-laboratory courses at Iowa State, for a required fluid mechanics sequence at Cornell, and for an aerodynamics course at Howard. Descriptions for Iowa, Iowa State, Cornell and Howard follow.

Iowa The introductory level fluid dynamics course at Iowa is a 4-semester hour junior level course required in Mechanical and Civil & Environmental Engineering and frequently elected by Biomedical Engineering students. Traditionally, course used 4-lectures per week for AFD with a few additional EFD labs for purpose of highlighting fundamental principles. Course restructured

for 3-semester hour AFD (3 lectures per week) and 1-semester hour (1 laboratory meeting per week) complementary EFD, CFD, and UA laboratories. EFD laboratories upgraded for present purposes and to include UA and achieve benchmark quality data, including tabletop viscosity, pipe flow stand, and wind tunnel airfoil flow experiments. As discussed herein, complementary CFD laboratories were developed. The course was also reorganized for web based teaching and distribution of materials <http://css.engineering.uiowa.edu/~fluids/>.

Educational goals for lectures, problem solving, and the EFD, CFD, and UA labs were developed and used as guidelines for course and laboratory development, implementation, and evaluation. Table 1 lists the general goal for the complementary EFD, CFD, and UA labs as well as the detailed goals for the EFD, CFD, and UA labs. Although CFD labs at Iowa used with complementary EFD and UA labs, also designed for *stand-alone* use. At Iowa, some instructors choose to follow more traditional approach to teaching introductory fluid mechanics course using 4 lectures on AFD per week and placing less emphasis on EFD UA and complementary CFD, i.e., use only portion of lab materials presented herein.

Table 1. Goals for complementary EFD, CFD, and UA labs

EFD/CFD and UA Labs General
1. Students will have <i>hands-on</i> experience with use of complementary EFD and CFD, including modern EFD, CFD, and UA methods and procedures, validate, analyze, and relate results to fluid physics and classroom lectures, and teamwork and presentation of results in written and graphical form.
EFD/UA Labs
1. Provide students with <i>hands-on</i> experience with EFD methodology and UA procedures through step-by-step approach following EFD process: setup facility, install model, setup equipment, setup data acquisition using labview, perform calibrations, data analysis and reduction, UA, and comparison CFD and/or AFD results.
2. Students will be able to conduct fluids engineering experiments using tabletop and modern facilities such as pipe stands and wind tunnels and modern measurement systems, including pressure transducers, pitot probes, load cells, and computer data acquisition systems (labview) and data reduction.
3. Students will be able to implement EFD UA for practical engineering experiments.
4. Students will be able to use EFD data for validation of CFD and Analytical Fluid Dynamics (AFD) results.
5. Students will be able to analyze and relate EFD results to fluid physics and classroom lectures, including teamwork and presentation of results in written and graphical form.
CFD/UA Labs
1. Provide students with <i>hands-on</i> experience with CFD methodology (modeling and numerical methods) and procedures through step-by-step approach following CFD process: geometry, physics, mesh, solve, reports, and post processing.
2. Students will be able to apply CFD process through use of educational interface for commercial industrial software to analyze practical engineering problems.
3. Students will be able to conduct numerical uncertainty analysis through iterative and grid convergence studies.
4. Students will be able to validate their computational results with EFD data from their complementary experimental laboratories.
5. Students will be able to analyze and relate CFD results to fluid physics and classroom lectures, including teamwork and presentation of results in written and graphical form.

A sequence of CFD, EFD, and UA labs developed to meet these goals. Labs intended for *hands-on* seamless teaching of CFD, EFD, and UA methodology and procedures as *tools* of engineering practice while at the same time relating results to fluid physics and classroom lectures. Table 2 provides an overview of the lab materials. During the first week of class, 1 classroom lecture is used to provide overview of AFD, EFD, and CFD as complementary *tools* of fluids engineering practice, which was followed throughout the semester by the AFD and problem solving lectures and EFD, CFD and UA labs. Students work in groups, but submit separate lab reports. EFD labs begin with lecture sequentially followed by viscosity, pipe flow, and airfoil flow experiments. Complementary CFD labs begin with lecture sequentially followed by pipe flow and airfoil flow simulations. Idea is for each lab to build on previous lab in sequence to achieve greater depth in each step of EFD or CFD process such that at advanced level students are nearly at level of engineering practice and additionally able to relate results to advanced fluid physics. Instructions provided for writing of lab reports, which constitute 25% of the final course grade. Instructions provided for each lab. Prelabs conducted for additional instruction. Students are also required to hand in answers to prelab questions to encourage their familiarity with lab materials before coming to the lab.

The class web site distributes the CFD lab materials. CFD lecture provides an overview of what, why, and where CFD is used, methodology (modeling and numerical methods), types of CFD codes, examples, and CFD educational interface. Lab report instructions guide students to write lab reports. Teaching assistants to grade the reports easily also use instructions. Different sections of lab report instructions are cross referenced to the Lab goals (Table 1), so the students' performances in the lab report can be used to provide evidence of students' skill and knowledge acquisition related to the lab goals. In Prelab 1, students were asked to learn how to run FlowLab following the CFD Process, be familiar with FlowLab interface, import and export data, and run simulation of laminar pipe flows with comparison to analytical solutions. In Lab 1, students conduct a more complicated case (turbulent pipe flow) and compare FlowLab predictions with their own EFD data obtained in EFD Lab 2. Students will simulate the inviscid flow around airfoil with different attack angles in PreLab 2 and conduct turbulent flow simulations on the same geometry in Lab 2 with validation by their own EFD data obtained in EFD Lab 3. Lab assignments use different options, such as investigations of effect of mesh refinement, effect of different turbulence models, and effect of different numerical parameters, etc. Students can choose the option that satisfies their interests the most. A companion paper at this conference describes EFD lab materials¹⁴.

Table 2: TM used for introductory fluid mechanics course at Iowa (EFD/CFD lab materials).

Lecture	Other Docs	Lab 1: Viscosity	Lab 2: Pipe Flow	Lab 3: Airfoil
EFD lecture	EFD UA Report Lab Report Instructions	Pre lab1 questions Lab1 lecture EFD 1	Pre lab2 Questions Lab2 lecture EFD 2 Lab2 UA:	LAB3 lecture EFD 3 Benchmark Data Data Reduction Sheet

		Lab1_UA Instructions_ UA	Smooth Rough Instructions_UA	Instructions_UA Combined EFD3/CFD2 report instructions
CFD Lecture	CFD lab report instructions	None	CFD Prelab1 CFD Prelab1 lecture CFD Prelab 1 questions CFD Lab 1	CFD PreLab2 CFD PreLab2 Lecture CFD Prelab2 questions CFD Lab2

Self-Evaluation As part of the overall evaluation process, a self-evaluation was performed based on analysis of the data from students' performance and comments from their EFD reports, college of engineering EASY survey, and Course Outcomes Assessments Administered by Center for Evaluation and Assessment data were analyzed. Most students' performance was very good, cooperative, and eager to learn. Students appreciated the *hands-on* learning process by using a step-by-step method through the educational interface, which enhanced their understanding of the CFD process to analyze and solve practical fluids engineering problems. The analysis also suggested several ways to improve implementation. (1) FlowLab: develop user-friendlier FlowLab interface and increase the depth of CFD templates. (2) Lab reports: combine the CFD and EFD lab reports and TA's lab reports grading is too liberal and does not break the grades to different categories as required by the lab report instructions. (3) Lab design: develop interactive and effective use of PreLab and Lab time. (4) Hands-on: provide more access to FlowLab and one-person one-computer to provide more *hands-on* experiences as required by students. Improvements planned for implementation for Fall 2004 for both introductory and advanced level CFD templates. The introductory level templates used for the current fluid class and the advanced level templates used for teaching an intermediate fluid class.

Iowa State Implementations conducted for aerodynamic sequence of courses and the gas-dynamic-laboratory course.

Aerodynamics I Lab The required aerodynamic sequence of courses at Iowa state are structured as incompressible potential flow (AERE 243. Aerodynamics I), compressible flow (AERE 311. Gas Dynamics) and viscous flow (AERE 343. Aerodynamics II).

Each of these courses is also strongly coupled with a lab course (AERE 243L. Aerodynamics I Lab, AERE 311L. Gas Dynamics Lab and AERE 343L. Aerodynamics II Lab respectively). The classes in general address AFD while the labs are used as EFD test-beds for certain concepts introduced in the class. CFD through the Fluent software was introduced in the first two labs Aerodynamics I Lab and Gas Dynamics Lab as part of the NSF project. In this paper we discuss the introduction of CFD (through the Fluent software) in Aerodynamics I Lab and Gas Dynamics Lab, and its impact on student learning in these courses.

Aerodynamics I Lab is a half a semester course and specifically discusses the following four concepts:

Concept 1. Streamlines, streak lines and path lines (AFD) and their connection to Flow visualization. Smoke tunnel is used in the EFD lab to visualize flow over two-dimensional and three-dimensional objects in the lab. Flowlab is introduced in this lab as a demonstration by the instructor. Snapshots from EFD and CFD are prosecuted below.



Fig. 3. Streamlines (experiment)

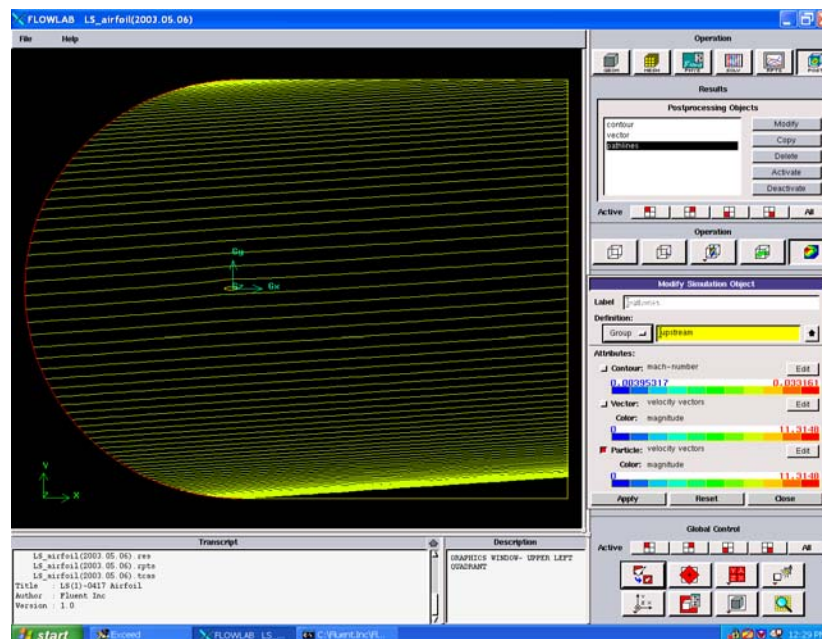


Fig. 4. Streamlines (FlowLab)

Concept 2. As an application of the Bernoulli's equation taught in the theory class a closed circuit wind tunnel is calibrated in the EFD lab.

Concept 3. Flow over a circular cylinder is introduced from the point of potential flow in the theory class. In the Lab course the pressure distribution over the 2-D cylinder is observed and contrasted with the potential flow solution. CFD use is required in this lab. The students are required to conduct the same experiments numerically using Flowlab and compare AFD, EFD and CFD results in the report they write. Examples from students work are presented in the following illustrations.

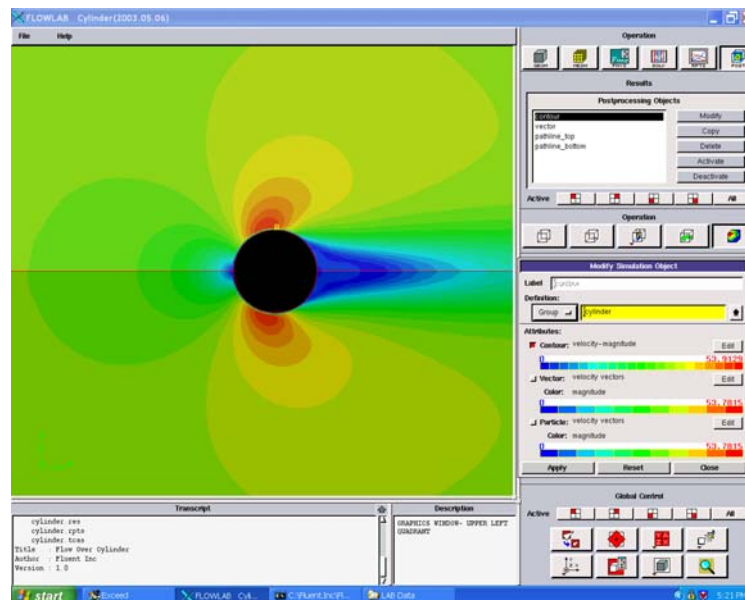


Fig. 5. Numerical results for the velocity magnitude distribution over a circular cylinder using FlowLab ($V_h=35.8$ m/s, $Re=1.89E+05$)

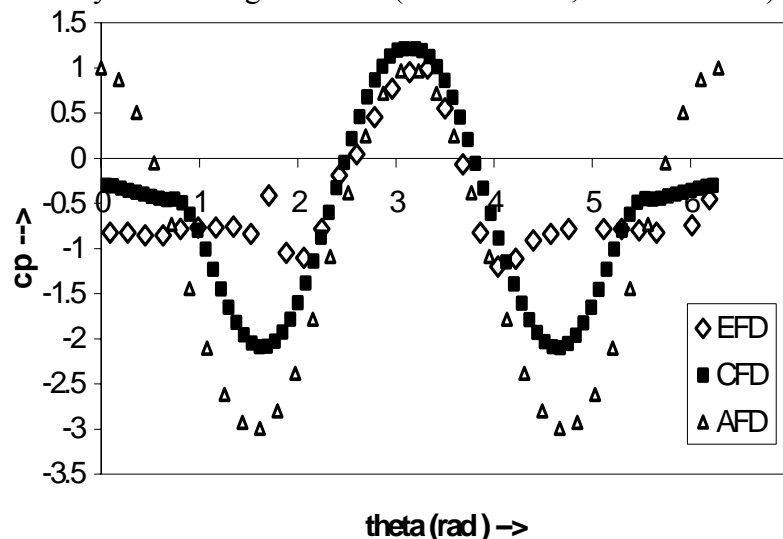


Fig. 6. C_p distributions over a circular cylinder

Aerodynamics I and the associated lab Aerodynamics I Lab are introductory courses and are sophomore level classes. CFD is introduced as a procedure for solving the partial differential equations that describe the flow. Students are encouraged at this level to become expert users of CFD through Flowlab, however, they are not required to know the details of the CFD theory.

Concept 4. The final lab involves the aerodynamic characteristics of an airfoil (C_l vs. α , C_d vs. α and C_m vs. α) using pressure measurement. Flowlab is used to conduct the same experiments numerically and pressure measurement comparison with EFD is presented in the following illustrations.

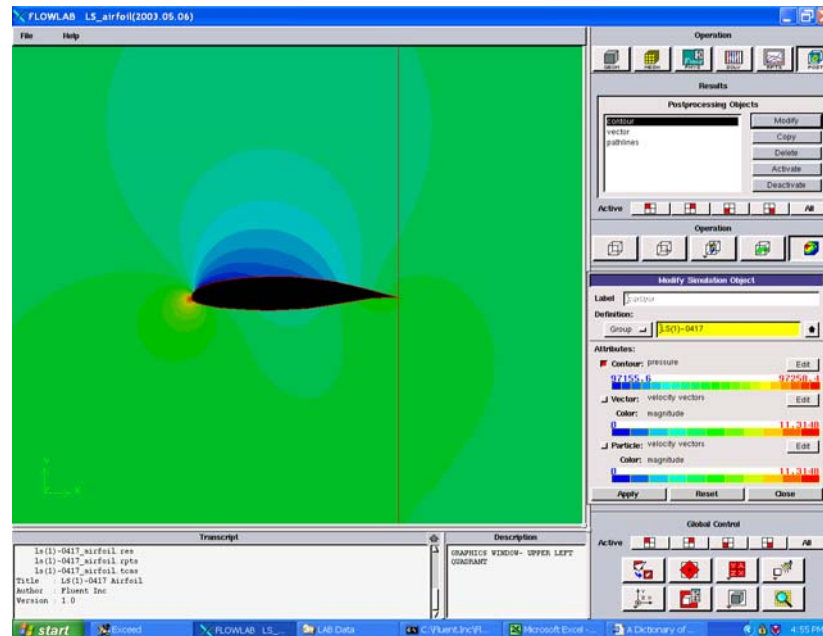


Fig. 7. Numerical results for the pressure distributions over LS(1)-0417 airfoil using the Flowlab (angle of attack=4 degree, $M_h=0.025$, $Re=2.0E+05$)

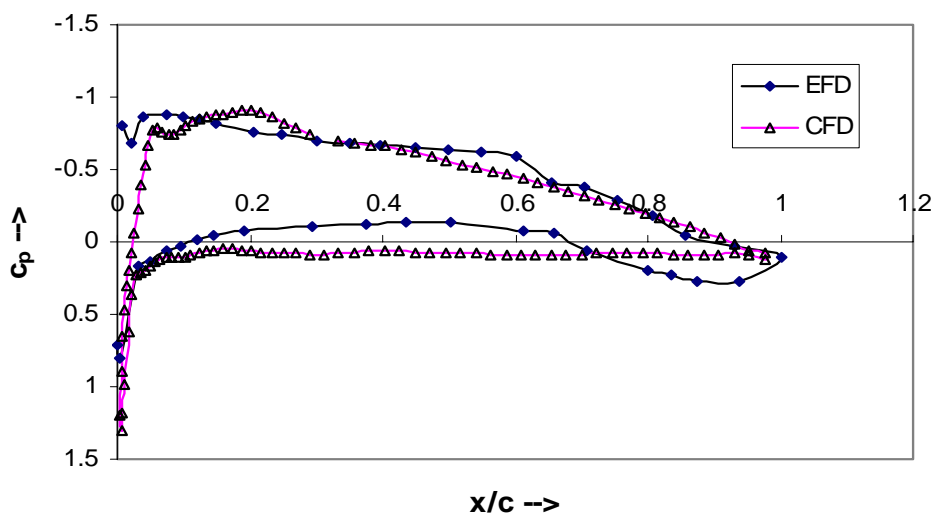


Fig. 8. C_p distributions over LS(1)-0417 airfoil

Table 3 Key results from AERO E. 243L survey								
Question		SA	A	a	d	D	SD	nop
Flowlab is an easy to use CFD tool.	n	1	10	12	3	1	2	0
	%	3	34	41	10	3	7	0
The hands-on aspects of the CFD lab helped me learn valuable skills and knowledge.	n	5	9	10	1	1	2	1
	%	17	31	34	3	3	7	3
CFD taught me things that I could not learn through EFD or AFD alone.	n	1	6	12	4	1	2	3
	%	3	21	41	14	3	7	10
The CFD lab contributed to my understanding of Aerodynamics.	n	4	5	16	2	0	2	0
	%	14	17	55	7	0	7	0
EFD and CFD results from this lab helped my understanding of AFD and the underlying theory.	n	1	7	16	1	2	1	1
	%	3	24	55	3	7	3	3
CFD is a useful addition to the EFD lab.	n	4	7	16	0	0	2	0
	%	14	24	55	0	0	7	0
I would recommend the CFD lab to others.	n	2	6	12	3	0	3	3
	%	7	21	41	10	0	10	10
I have used CFD in some form before this class.	n	5	2	2	4	3	12	1
	%	17	7	7	14	10	41	3
As a result of my learning in this course, I have run one or more simulations with Flowlab.	n	9	7	12	1	0	0	0
	%	31	24	41	3	0	0	0
As a result of my learning in this course, I can appreciate the connection between EFD, AFD & CFD.	n	8	10	9	0	1	0	1
	%	28	34	31	0	3	0	3
As a result of my learning in this course, I have a basic understanding of CFD methodology and procedures.	n	3	6	12	5	1	1	1
	%	10	21	41	17	3	3	3

The gas-dynamics-laboratory course The gas-dynamics-laboratory course taught at Iowa State University is a junior level course. This 0.5 credit hour course complements a 3-credit hour lecture course. Being taught in the second half of the semester, the laboratory course reviews the theory, and introduces experimental procedure and CFD analysis using Flowlab.

The first experiment taught in the course examines the time evolution of pressure and temperature in the blowdown of a high pressure tank. The second experiment considers wall pressure measurements for different shock positions within a nozzle which is connected to the tank. As air is blown through the nozzle, there is gradual change in the observed flow patterns, from expansion fans through oblique shocks and normal shocks within the nozzle. Students examine the 1st, 2nd and 3rd criticals for the nozzle using a combination of experiment, theory and CFD. The 1st critical refers to the case when the throat Mach number is 1, 2nd critical for a standing shock at the nozzle exit and 3rd critical for a smooth flow devoid of shocks and expansion fans.

Bearing in mind that the class met once every week for seven weeks of the semester, the first two weeks of the class were used to acclimatize students to the Schlieren method of flow visualization as well as to present an overview of the one-dimensional nozzle theory. In the third week, the first blowdown experiment was performed in groups of 4 students. An introduction to

CFD using Flowlab was given in the third week. The lecture consisted of an overview of CFD methods and Flowlab, accompanied by a tutorial section for each segment – such as defining physics, creating mesh and solving for the result. The objective of the CFD lecture was to emphasize the actual CFD decision making process when using Flowlab.

A second CFD lecture was given in the fourth week, along with CFD practice sessions. The second CFD lecture covered additional physics and mathematics, such as the need for grid stretching and the properties of shock boundary-layer interactions. The second experiment as well as CFD exercises were performed in the fifth and sixth weeks. The second experiment involved measurement of wall pressure for six cases: under-expanded flow, 3rd critical, over-expanded flow with oblique shock, 2nd critical, shock between throat and exit of the nozzle, and 1st critical. The second CFD exercise consisted of two parts. In the first part, the students reproduced one of the cases from the experiment. In the second part, the students used a tank pressure value between 1st and 2nd critical to create and visualize a λ -shock.

The CFD solutions from Flowlab were found using a nozzle template developed by Fluent. Close interaction between Iowa State and Fluent resulted in a template which provided acceptable comparison with experiment as well as reasonable run times.

The Flowlab template for the nozzle was designed to use three types of meshes with varying degrees of mesh density: coarse, medium, and fine. All of these meshes take into account the presence of the boundary layer. The primary control parameters for the simulation are inlet total pressure and the flow model (e.g. inviscid, laminar or turbulent). Two flow geometries were used in our class (axisymmetric and 2D). A complete 3D calculation for the rectangular cross-section nozzle which was actually used in the experiment would take more time than we deemed to be acceptable.

The CFD exercises for Flowlab were tested using a computer with 512 MB RAM and an Intel Pentium 4 1.8 GHz processor. Students performed the Flowlab exercises in a departmental computer lab with computers which had two 866 MHz Pentium III processors and 512 MB RAM.

As seen in Table 4, it was observed that most of the cases had run times of 10-20 minutes when using the medium mesh configuration and an inviscid model. Fine mesh cases took 1.5 to 2 times longer than the medium mesh configurations. The run times for 2D and axisymmetric cases were similar. However, some cases involving inviscid flow took a long time for convergence. For example, when a plenum was added to the nozzle exit between 1st and 2nd criticals, and inlet total pressure was 170000 Pa, the time taken for convergence was more than the case without the plenum and same inlet pressure. This time was also more than the time taken for a case with plenum and inlet total pressure close to 2nd critical. It should also be noted that the λ -shock case exhibited strong oscillatory behavior in convergence. In addition, the λ -shock from Flowlab was seen to be larger than the shock observed in the experiment.

Table 4. Flowlab run times with medium mesh				
Inlet pressure	Flow model	Run time (in minutes)	Number of iterations (approx)	Convergence Limit
114845 Pa – (1 st critical – From expt. = 108,220 Pa)	Inviscid	5	230	10 ⁻³
250000 Pa ⁺ – (2 nd critical – From expt. = 253,010 Pa)	Inviscid	15	1100	2x10 ⁻³ *
450000 Pa ⁺ – (3 rd critical – From expt. = 446,063 Pa)	Inviscid	9	315	10 ⁻³
163000 Pa – λ -shock	Turbulent (k- ϵ)	23	1550	10 ⁻³

* - iteration usually required interruption, since the residual for continuity oscillated around this number.

+ - based on visual examination

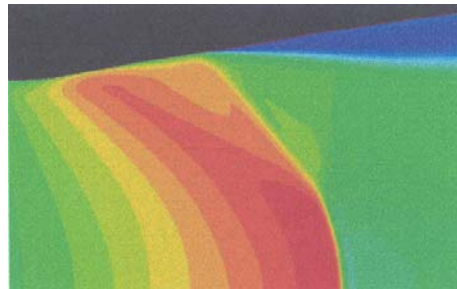


Fig. 9. Typical Mach number contour for a λ -shock using Flowlab.

A Mach number contour from a student's report is shown in Fig. 9. In this figure, the Spalart-Allmaras model was used as the turbulence model. An inlet total pressure of 165,000 Pa and an outlet pressure of 1 atm were used, which produced a shock in the diverging section of the nozzle.

A course survey was conducted and administered by the University of Iowa. Some of the key results are presented below. In this table, n is the number of students, and AFD and EFD refer to analytical and experimental fluid dynamics, respectively.

Table 4.1 Scales used in survey						
Strongly Agree	Moderately Agree	Mildly Agree	Mildly Disagree	Moderately Disagree	Strongly Disagree	No Opinion
SA	A	A	d	D	SD	nop

Table 4.2 Key results from survey								
Question		SA	A	A	d	D	SD	nop
Flowlab is an easy to use CFD tool.	n	2	10	11	3	0	3	0
	%	6.90	34.48	37.93	10.34	0	10.34	0
The hands-on aspects of the CFD lab helped me learn valuable skills and knowledge.	n	3	7	12	5	1	1	0
	%	10.34	24.14	41.38	17.24	3.45	3.45	0
CFD taught me things that I could not learn through EFD or AFD alone.	n	2	6	11	6	0	0	4
	%	6.90	20.69	37.93	20.69	0	0	13.79
The CFD lab contributed to my understanding of Aerodynamics.	n	1	11	10	5	0	1	1
	%	3.45	37.93	34.48	17.24	0	3.45	3.45
EFD and CFD results from this lab helped my basic understanding of AFD and the underlying theory.	n	1	9	13	3	1	1	1
	%	3.45	31.03	44.83	10.34	3.45	3.45	3.45
CFD is a useful addition to the EFD lab.	n	6	6	11	4	0	1	1
	%	20.69	20.69	37.93	13.79	0	3.45	3.45
I would recommend the CFD lab to others.	n	3	9	11	4	1	1	0
	%	10.34	31.03	37.93	13.79	3.45	3.45	0
I have used CFD in some form before this class.	n	2	4	9	2	3	8	1
	%	6.90	13.79	31.03	6.90	10.34	27.59	3.45
As a result of my learning in this course, I have run one or more simulations with Flowlab.	n	8	11	7	2	0	0	1
	%	27.59	37.93	24.14	6.90	0	0	3.45
As a result of my learning in this course, I can appreciate the connection between EFD, AFD & CFD.	n	8	12	7	1	0	0	1
	%	27.59	41.38	24.14	3.45	0	0	3.45
As a result of my learning in this course, I have a basic understanding of CFD methodology and procedures.	n	5	14	6	2	0	1	1
	%	17.24	48.28	20.69	6.90	0	3.45	3.45

In the survey, it was found that most of the responses were around ‘A’ and ‘a’. The questions for the assessment of work done for the lab reports received ‘SA’ and ‘A’ responses, which meant that most students had participated in preparing the lab reports. Responses to CFD related questions, which are tabulated above, indicate that students indeed benefited from the usage of Flowlab.

Though most students assessed the volume of material covered to be correct, there were a few students who observed that the Flowlab exercises took too long to complete. However, most of the students appreciated having the CFD component in the course and felt that having all three components of fluid flow analysis, i.e. EFD, AFD and CFD, led to better understanding of the course material.

Cornell The pipe flow template was used in a required senior-level fluid mechanics and heat transfer lab course. The class had 110 students with 2 professors and 6 teaching assistants providing instruction. The lab was taught in small groups of 6-8 students. The lab experiment involved turbulent flow of air through a smooth-walled copper pipe duct consisting of three sections. The first section was unheated and generated a hydrodynamically fully-developed turbulent velocity profile, the middle section was heated providing energy input to the air, and

the final section was insulated providing an adiabatic mixing length to allow a single or bulk reading of the final air temperature. The apparatus was equipped with instrumentation for measuring (1) air mass flow rate, (2) pressure drop over a given length, (3) temperature distribution along the duct wall and temperature rise of the air, (4) temperature profile at the exit of the duct, and (5) energy input to the heating ribbon. In previous years, this lab involved operation at one heated condition (corresponding to a single Reynolds number and Nusselt number) and several unheated conditions. In order to accommodate complementary numerical simulations using FlowLab, the lab was modified to include operation at one heated condition only with operation at the unheated conditions being dropped.

In the first week of the lab for each student group, the instructor introduced the experimental set-up and data acquisition as well as the pipe flow template. The hands-on template introduction involved each student following directions from the instructor for simulating the heated pipe flow using sample input data. This was done in a computer lab adjacent to the experimental apparatus. In the second week, data processing was discussed in a recitation session. The lab report was due a week after that. Students were provided with a handout that discussed (1) the basic strategy of CFD, (2) the CFD solution process, (3) the details of stepping through this process in the pipe flow template, (4) background on turbulence modeling, and (5) operating details of running FlowLab, such as controlling the graphical display and exporting files into Excel, and using the computer lab. This handout will be made available on the FlowLab website as an example for interested instructors at other universities.

In their reports, students were required to compare the friction factor and Nusselt number obtained from their experiment with corresponding values from their FlowLab simulation and correlations in the literature. A typical comparison of the results for a Reynolds number (based on pipe diameter) of 100,820 is shown in Table 5. The simulation results compare reasonably well with those from experiment, with the difference in friction factor and Nusselt number being 7% and 4%, respectively.

Table 5: Typical results for the pipe flow lab at Cornell university.

	Experiment	Simulation	Correlation
Friction factor	0.0180±0.003	0.0168	0.0177
Nusselt no.	185	192	183

The pipe flow template enabled students to visualize velocity vectors and the temperature field which helped them gain a better physical understanding of the experimental system than is possible from a few point measurements. This was noted by a majority of students in their course evaluation. The template helped them appreciate that numerical modeling involves approximations and tradeoffs. The simulations were used to confirm some of the assumptions made in data reduction for the experiment, for instance, that the adiabatic mixing region is long enough for the temperature to be uniform at its exit. The template results provided confirmation of the experimental and correlation results, and showed how these approaches can complement each other.

We worked closely with personnel at Fluent Inc. to insure that the pipe flow template met the requirements at Cornell. For example, a feature enabling specification of constant heating along a specified subsection of the pipe was added at our request. There were some early problems with the template that resulted in program crashes and poor agreement with experiment. Fluent Inc. personnel paid a visit to Cornell to discuss the problems and responded in a timely fashion to fix them before student use of FlowLab. Our experience was that small groups were well-suited to introducing students to CFD basics through FlowLab. The FlowLab experience resulted in many students showing an enthusiasm for learning more about CFD.

Howard The airfoil and pipe flow templates were used in a required, junior-level fluids mechanics course (MEEG 307). There were 15 students in the class and the students were divided into groups of three. The simulation component of the course began with an introduction to CFD and error analysis. The students then used the templates and FlowLab in open-ended homework problems and as a design tool for laboratory experiments for the following semester. Unlike at the other partner institutions, the fluids/thermal laboratory component at Howard University occurs in the second semester. The formal assessment will be performed in the spring semester when we incorporate the EFD component of the project. However, informally we received a positive response from students and the suggestion that the simulation be introduced earlier in the semester. The course may be redesigned for the Fall 2004 semester if the responses are similar for the companion course.

Evaluation

The evaluation design treats each of the four sites as separate case studies applying instructional techniques and software in the context of different curricula at the different sites¹⁵. Course goals at each site are related to the ABET standards, but are expressed in terms of the general engineering course goals and objectives at each site.

The guiding evaluation questions addressed by this design are the same at each site:

- Were student learning needs met and did the students benefit from the implementation of the CFD software and instructional interfaces? If so, in what ways did they benefit? If not, why not?
- In what ways can the efficiency or the effectiveness of the CFD products and implementation be improved?
- What are especially important strengths of the current implementations that need to be maintained in the next year or for future implementations at other schools and colleges of engineering.

Methodology The methodology used in this evaluation design envisioned three primary sources of information:

1. Faculty and Teaching Assistant judgments of the quality of lab reports and/or of exam results.
2. Student responses to independent, anonymous survey items asking them to judge their own learning from specific instructional components in retrospective fashion, a method with investigated and documented validity for low stakes judgments¹⁶.
3. Student responses to independent, anonymous survey items asking them to provide evaluations of all the separate implementation components and to comment on how to improve the efficiency and effectiveness of the implementation, especially *hands-on* components

The survey items were developed separately for each university site and collaboratively with faculty from each site. Students responded to the survey items during the last week of class with anonymity and without the instructor present. Site IV will participate in future data collection. Surveys included some shared items, but focused primarily on the tailored instructional goals at each site. Complete versions of the surveys as administered are available as PDF files at the following Web site: <http://www.iuhr.uiowa.edu/~istue/>. Open-ended survey items requested respondent comments. Students were also asked to respond to direct statements indicating their degree of agreement or disagreement (e.g., “This course increased my interest in fluid mechanics” or “As a result of my learning in the CFD labs, I am able to present results from CFD simulations in written and graphical form). Respondents were asked to agree or disagree on a six point Likert type scale ranging from “strongly agree” (scored as 6) to “strongly disagree” (scored as 1) scale. Respondents with insufficient information or who otherwise did not want to respond could choose a “no opinion” response.

Results for the Site I implementation Student lab reports At Site I, lab reports were originally scored for general quality and learning outcomes as part of the grading process. After the end of the grading process, a post-doctoral associate and the PI analyzed the lab reports to document the extent to which student lab reports provided evidence of students’ skill and knowledge acquisition related to the CFD implementation goals. The evaluation team is currently reviewing these procedures and analyses to investigate their reliability and generalizability (validity).

Table 6 presents the percentage of students at the Site I implementation whose lab reports indicated that specific instructional goals had been achieved.

Table 6: Percentages of lab reports providing evidence of specific goal attainment, as judged by the course instructor and teaching assistants

Goals	Student Performance		Reports Sections
	Lab1	Lab2	
1. Provide students with <i>hands-on</i> experience with CFD methodology (modeling and numerical methods) and procedures through step-by-step approach following CFD process: geometry, physics, mesh, solve, reports, and post-processing.	96%	96.5%	Total
2. Students will be able to apply CFD process through use of educational interface for commercial industrial software to analyze practical engineering problems.	100%		3
3. Students will be able to conduct numerical uncertainty analysis through iterative and grid convergence studies.	N/A		4
4. Students will be able to validate their computational results with EFD data from their complementary experimental laboratories.	100%		3,4
5. Students will be able to analyze and relate CFD results to fluid physics and classroom lectures, including teamwork and presentation of results in written and graphical form.	91%		4,5

Site I Survey Responses. For purposes of this report, survey items were categorized into clusters addressing the following topics:

- General Learning Needs Met by the Course (23 items, for example: “My learning needs were well met in this course”, “The information in this course was presented effectively”
- Hands-on aspects of the CFD Component (2 items: “The hands on aspects of the Computational Fluid Dynamics Lab helped me learn valuable skills and knowledge”, “The hands-on aspects of the Computational Fluid Dynamics Lab worked well for me”
- Skills and Knowledge Gained Using the CFD Component (10 items: “As a result of my learning in the CFD Lab, I am able to use Flowlab for solving laminar and turbulent pipe flow and inviscid and viscous airfoil flow”, “As a result of my learning in the CFD Lab, I am able to evaluate grid convergence through analysis of solutions on coarse, medium, and fine grids.

Table 7 lists the items included in each cluster score. All cluster scores were investigated to determine their reliability¹⁷. Table 7 presents the internal consistency reliability estimates of the three cluster scores as well as their simple Pearson product moment correlations with each other.

Table 7. Cluster score reliability estimates and product moment intercorrelations

	Learning Needs Overall	Hands-On CFD	Skills, Knowledge Gained CFD
Learning Needs Overall	.94 ^a (54)		
Hands-On CFD	.58 (54)	.92 ^a (54)	
Skills, knowledge Gained CFD	.64 (54)	.74 (54)	.95 ^a (55)

Note. Numbers in parentheses indicate the number of cases from a total of 62 students who provided some survey information. ^aCronbach's Alpha reliability coefficients

As can be seen in Table 7, all cluster scores showed high reliability estimates and moderate correlations with each other, suggesting that they provided good measures of the named constructs, and that respondents were able to differentiate the three constructs from one another. For example, the R^2 for the simple correlation of the cluster score "Hands-On Aspects of CFD" with the cluster score "Learning Needs Met Overall" ($R^2 = .64$ squared = .40) suggested that only about 40% of the variance in students' responses to the items constituting one of these cluster scores can be explained by students' responses to the other cluster score.

Of greater interest for the evaluation of the CFD implementation are the averages and distributions of students responses to the items clustered into these constructs. In general, the more strongly the students agreed with these items (or disagreed with the reverse, negatively stated items) the more support they were expressing for the extent to which their overall learning needs were met, for the quality of the hands-on components, or for the knowledge and skills gained from the CFD implementation.

Table 8 presents the means and standard deviations for each of these three cluster scores. Cluster scale scores are the sum of all scale item responses divided by the number of items in that cluster in order to give the cluster scores for each individual the same range and anchors (6=Strongly Agree, 1=Strongly Disagree).

Table 8. Cluster score means and standard deviations

Scale	<i>N</i> Cases	<i>N</i> Items	Mean	SD	Minimum	Maximum
Learning Needs Overall	55	24	4.56	0.65	2.81	5.63
Hands-on CFD	55	2	3.44	1.36	1.00	6.00
Knowledge, Skills CFD	55	11	4.40	0.93	2.00	6.00

As can be seen in Table 8, respondents on average "mildly to moderately" agreed that their overall learning needs were met ($M=4.56$ out of a possible 6.0, $SD=.65$) and "mildly to moderately" agreed that their knowledge and skills improved as a result of the CFD lab ($M=4.40$,

SD=.93). However, students on average were not in agreement with statements about the quality of the *hands-on* experience in the CFD lab either helped them learn valuable skills and knowledge or worked well for them ($M=3.44$, between “mildly agree and mildly disagree”, $SD=1.36$). The variability of cluster scores was great: individual student cluster score responses ranged from strongly disagree to strongly agree. Thus on all cluster scores, some students appeared to be well-satisfied with these efforts while others appeared to be in strong disagreement that these CFD implementation efforts were effective for them.

Students were also given the opportunity to respond to open ended survey items elaborating on their evaluations of the CFD labs and the hands-on components of the labs. In response to the question: “In your own words, what are the best things about learning with the CFD lab?”, 59 of 62 students provided comments. Two raters independently categorized all comments into one or more of 7 categories (overall rater agreement, $Kappa = .76$), listed below.

Useful, new understanding/knowledge: 10 responses. For example, respondents mentioned the speed of getting results helped learning, that they appreciated learning the new software, and that they were acquiring “knowledge of a program that is being used in many businesses...will be a good tool in the future.”

Quality of the hands-on aspects: 7 responses. For example, students mentioned that “the hands on aspect is best”...getting to see graphical data, using the software to understand what is going on in a flow, seeing what you learned in the lecture, and being able “to use technology instead of raw equations to obtain answerable solutions.”

Quality of the software capabilities: 13 comments. Students mentioned the visual operating format that “combines multiple data processing programs”, the graphs, ability to change the angle of attack for airfoil experiments, ability to impact any parameter and see the output instantly, ability to pick questions, experiments and factors of individual interest, and ease of set-up and error correction.

Value of visualization of results: 14 comments. Students commented on the power of the graphical presentations to make the output interesting and meaningful. Several indicated this was the best thing about the CFD. Several thought the post processing visualization was useful in understanding what was going on.

Value of instruction or teaching, 7 responses. Students commented on TAs being helpful and on the usefulness of the step-by-step approaches.

Miscellaneous negative comments: 7 comments. Even though this question asked for benefits, seven respondents indicated that they did not benefit, found the software confusing and unhelpful, or were not able to learn from the TAs.

In response to the question: “What needs to be improved in the CFD lab to maximize its value to you?”, 59 students out of 62 provided comments. Two raters independently categorized all comments into one or more of three categories below (overall rater agreement, $Kappa = 0.72$).

Increased access/individual use: 10 comments. Students wanted more computers so that individual access to the keyboard for everyone would be possible.

Technical aspects/software: 7 comments. Students complained about the physical facilities, the colors on the screen, computers locking up, and especially unfriendly user interfaces.

Instruction/organization: 30 comments. Students wanted better organization, clearer instructions and guides, better understanding of what specific things mean, better collaboration between the experimental flow lab and the CFD, smaller groups, more time to learn and more long-term integrated projects, better instructions, and so forth.

Site II Results At Site II, no lab reports were analyzed. However, extensive open ended and Likert type items were administered to students in the fluid dynamics course. For purposes of this report, the Likert type survey items were categorized into clusters addressing the following topics three topics.

- General Learning Needs Met by the Course: (23 items, for example: “My learning needs were well met in this course”, “The information in this course was presented effectively”)
- Knowledge and Skills acquired through the CFD Component: (12 items: “CFD taught me things that I could not learn through EFD or AFD alone”, “I can relate CFD results to fluid physics presented in the lecture course”).
- Quality of the Hands-On Components: (2 items: “The hands-on aspect of the CFD lab worked well for me”, “The hands-on aspects of the CFD Lab helped me learn valuable skills and knowledge”).

Table 9 lists the items included in each cluster. All cluster scores were investigated to determine their reliability¹⁷. Table 9 presents the internal consistency reliability estimates of the three cluster scores as well as their simple Pearson product moment correlations with each other.

Table 9. Cluster score reliability estimates and product moment intercorrelations for Iowa state university.

	General Learning Needs	Hands-On CFD	CFD Knowledge & Skills
General Learning Needs	.95 ^a (28)		
Hands-On CFD	.53 (28)	.89 ^a (28)	
CFD Knowledge & Skills	.62 (28)	.67 (28)	.95 ^a (28)

Note. Numbers in parentheses indicate the number of cases from a total of 28 students who provided some survey information. ^a Cronbach’s Alpha reliability coefficients

Similar to the data summaries from Site I, these correlations and internal consistency estimates indicate that the cluster scores are measuring somewhat different constructs and display a high level of internal consistency reliability.

Also at Site II, of greater interest are the measures of central tendency and variability for the cluster scores. Table 10 presents the means and SDs for these three cluster scores.

In general, the more strongly the students agreed with these items (or disagreed with the reverse, negatively stated items) the more support they were expressing for the extent to which their overall learning needs were met, for the quality of the hands-on components, or for the knowledge and skills gained from the CFD implementation.

As before, cluster scale scores are the sum of all scale item responses divided by the number of items in that cluster (in order to give the cluster scores for each individual the same range and anchors, 6=Strongly Agree, 1=Strongly Disagree).

Table 10. Cluster score means and standard deviations

Scale	<i>N</i> Cases	<i>N</i> Items	Mean	SD	Minimum	Maximum
General Learning Needs	29	12	4.20	0.85	2.12	5.65
CFD Knowledge & Skills	29	12	4.62	1.07	1.00	5.63
Hands-On CFD	29	2	4.14	1.06	1.00	5.50

As can be seen in Table 10, respondents on average “mildly to moderately” agreed that their overall learning needs were met ($M=4.20$ out of a possible 6.0, $SD=.85$) and “mildly to moderately” agreed that their knowledge and skills improved as a result of the CFD lab ($M=4.62$, $SD=.1.07$). In addition, students on average mildly agree that the quality of the *hands-on* experience in the CFD lab either helped them learn valuable skills and knowledge or worked well for them ($M=4.14$, $SD=1.06$). It’s important to note that the variability in all of these cluster scores was great, and that individual student cluster score responses ranged from strongly disagree to strongly agree. Thus on all cluster scores, some students appeared to be well-satisfied with these efforts while others appeared to be in strong disagreement that these CFD implementation efforts were effective for them.

Students were also given the opportunity to respond to open ended survey items elaborating on their evaluations of the CFD labs. In response to the question: “In your own words, what about the CFD component worked especially well for you or was especially beneficial to you?”, 25 of 29 students provided comments. Two raters independently categorized all comments into one or more of four categories (overall rater agreement, Kappa = 0.72):

Quality of the Hands-On Component: 6 comments. Students commented that they liked the hands-on nature of the CFD lab and that they liked practicing it.

Value of Visualization of Results: 9 comments. Students commented that it was “nice to see the physical data showing shocks” or that it was valuable to see “the flow move as a result of changes in inlet and outlet pressure,” and/or that obtaining and seeing the many different contours was valuable.

Ease of Use: 5 comments. Five respondents commented that the CFD was easy to use.

Negative Comments: 3 comments. Three respondents provided negative comments even though the survey question asked for the useful and beneficial aspects. One said that there was not enough time spent on setting it up; another said that it was a waste of time when it “blew up.” The third said that the best thing about it was “when it was over”.

Students also responded to the question: “In your own words, what about the CFD component should be changed the next time it is taught? What needs to be improved?” 21 of 29 student respondents provided comments, which two raters then categorized into one of two categories ($Kappa = 0.72$).

Changes to technical aspects: 8 comments. Students said that Flowlab bugs needed to be fixed, that the software needed to be fixed, that it needed to be easier to print, and that occasionally Flowlab gives results that were not anywhere close to those obtained from real experiments.

Changes to instruction and teaching: 13 comments. Respondents listed a number of areas that needed improvement, including specific topics, for example, more clearly explaining the viscous modeling and designing manual meshes. More general comments included “...more time spent explaining Flowlab and setting it up”, or requesting more instruction, or asking for less lecturing or more lecturing. Two comments requested more hands-on time. One student thought that Flowlab was more trouble than it was worth and not very dependable, asking instead that “Fluent should be taught directly”.

Results from the Site III implementation The survey administered at Site III was shorter than the other surveys and only addressed the CFD component. Nine Likert type scale items, scored as described previously, addressed the knowledge and skills acquired. These items all began with the stem, “As a result of my learning in the CFD Labs, I am able to” and continued with such statements as “present results from CFD simulations in written and graphical form,” or “run Flowlab and implement CFD process for laminar and turbulent flow.” The average over all items for 77 of 80 responding students was 4.16 ($SD = 1.15$ students), indicating that students, on average, “mildly agreed” with these statements. Strongest agreement ($M=4.63$, $SD = 1.16$) was for the item, “...I am able to appreciate that simulation involves approximations and tradeoffs”. Least agreement, ($M=3.68$, $SD = 1.20$, between “mildly agree” and “mildly disagree”) was for the item, “...I am able to evaluate iterative convergence through setting iterative convergence criteria and analysis of solutions residuals.” As with the other institutions, the most striking aspect of the responses is the variability, ranging from “Strongly Disagree” to “Strongly Agree” on all items.

Students were also given the opportunity to respond to open ended survey items elaborating on their evaluations of the CFD labs. In response to the question: “In your own words, what are the best things about learning in the CFD lab, 58 of 81 students commented. Two raters independently categorized all comments into one or more of five categories (overall rater agreement, Kappa = 0.72):

Increases in understanding and knowledge: 15 comments. Students’ responses included the value of learning the software and the interface, learning the theory modeled by the software, comparing the CFD to the experimental results, learning more about simulation, learning about flow and how to plot out results, and learning about the trade-offs and limitations.

Quality of the hands-on aspects: 6 comments. Respondents commented on the value of getting to try out the concepts that they were learning and actually run the software themselves.

Capabilities of the software: 6 comments. Students listed particular strengths of the software and learning with the software, including the capability to change parameters and run new simulations quickly, producing thorough and clear output, and the complexity that allowed many ways to make mistakes from which one could learn. One comment emphasized that the colors were pleasant and that the interface was friendly. Another like the ease with which the error analysis section could be reported.

Visualization of results: 17 comments. All 17 commented on the benefit of being able to visualize the flow and/or contours and seeing this as helpful.

Miscellaneous negative comments: 8 comments. Two respondents mentioned that they already had CFD experience and didn’t benefit much from this introduction. Others thought this experience was too complicated, too brief, or would not generalize to other settings where they had to use the real software. One commented that the obtained results were not accurate.

Students at Site III also had the opportunity to respond to the question: “What needs to be improved in the CFD lab to maximize its value to you? Forty one students out of a total of 81 respondents provided comments. Two raters categorized the comments into the following four categories.

Technical aspects: 8 comments. Four respondents complained that their grids did not converge. Others mentioned that the software was buggy, requested better post processing and resizing techniques, and commented that the “saving” procedure was tricky.

Instruction and Teaching: 26 comments. These respondents provided numerous suggestions for improvement, including better trained and more knowledgeable TAs, better instructions and instruction booklets, more tutorials on CFD, a more vigorous approach with more time spent, perhaps in a workshop but not in this course, better explanations of how variables affect the output, more emphasis in lab reports and more time spent on learning the principles.

Time Issues: 7 comments. All six requested that more time be spent on CFD. One said if more time cannot be allocated then don't include it at all.

Miscellaneous: 3 comments. Two stated that they preferred to learn Fluent rather than Flowlab. One commented on the lack of student control and wanted to do more than just plug in numbers.

Evaluation Conclusions The evaluation results indicate that considerable progress has been made toward developing implementations that accomplish some of the learning goals. In addition, the implementation is improved in numerous ways over the Year One efforts. In spite of this improvement, there remain numerous areas where the Flowlab implementation can be improved for the majority of students like these. These possible areas of improvement are outlined below.

One important characteristic to be explored in future data collections is the variability in student responses. Students varied greatly in their appreciation of the CFD experience, with some reporting considerable growth and learning and others reporting frustration and lack of benefit. Future data collections will examine how the students who express benefit from the CFD experience are different from students who are frustrated and do not seem to benefit from the CFD component. It may be that the implementation can only be improved so much and that some students will continue to benefit while others do not. The fact that this variability exists across the three varied sites suggests that it is not an artifact or one pool of learners but is rather characteristic of fluid dynamics courses more generally. Future studies will investigate and report the student characteristics that correlate with benefiting from the CFD lab/component compared with characteristics of those students who do not benefit.

Conclusions and Future Work

Project is successful in development of CFD educational interface for pipe, nozzle, and airfoil flows, including design for teaching CFD methodology and procedures, implementation based on site testing at partner universities with different courses or laboratories, applications, conditions, exercise notes, and evaluations. Site testing indicates versatility of CFD educational interface since courses and pedagogy different at different universities, which suggests wider applicability of CFD educational interface at diverse universities. Evaluation indicates areas of strength as well as strategies for improvements and more effective implementation. Future work will focus on the following improvements. (1) Develop improved user interface: dynamic sketch window, import and export data, etc., reports (convergence histories, separate monitoring convergence from diagnostics results), diagnostics capabilities and graphics, including verification and validation. (2) Develop extensions for additional active options and advanced level (See Fig. 10 and Fig. 11). (3) Develop extensions for more general wider applications CFD templates: for internal (pipe, transition, low and high speed, heat transfer, noncircular cross section) and external (2D, 2D unsteady, 3D, 3D unsteady) flow. (4) Develop extensions for student individual investigation/discovery. (5) Use smaller lab groups with emphasis *hands-on* activities and remote access via college computer labs and Internet. (6) Perform implementation (with improvements) and site testing and evaluation. (7) FLUENT will disseminate current TM.

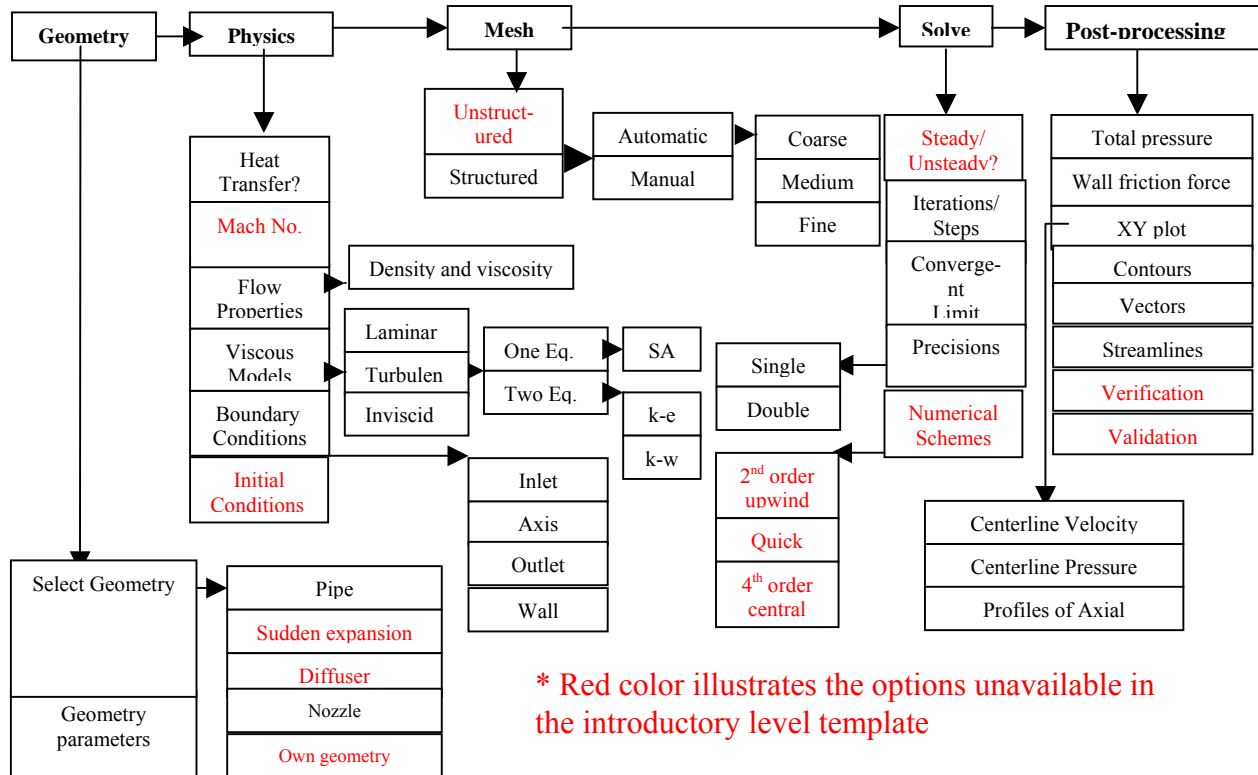


Fig. 10. Flow chart for combined 2D axisymmetric advanced internal flow template*

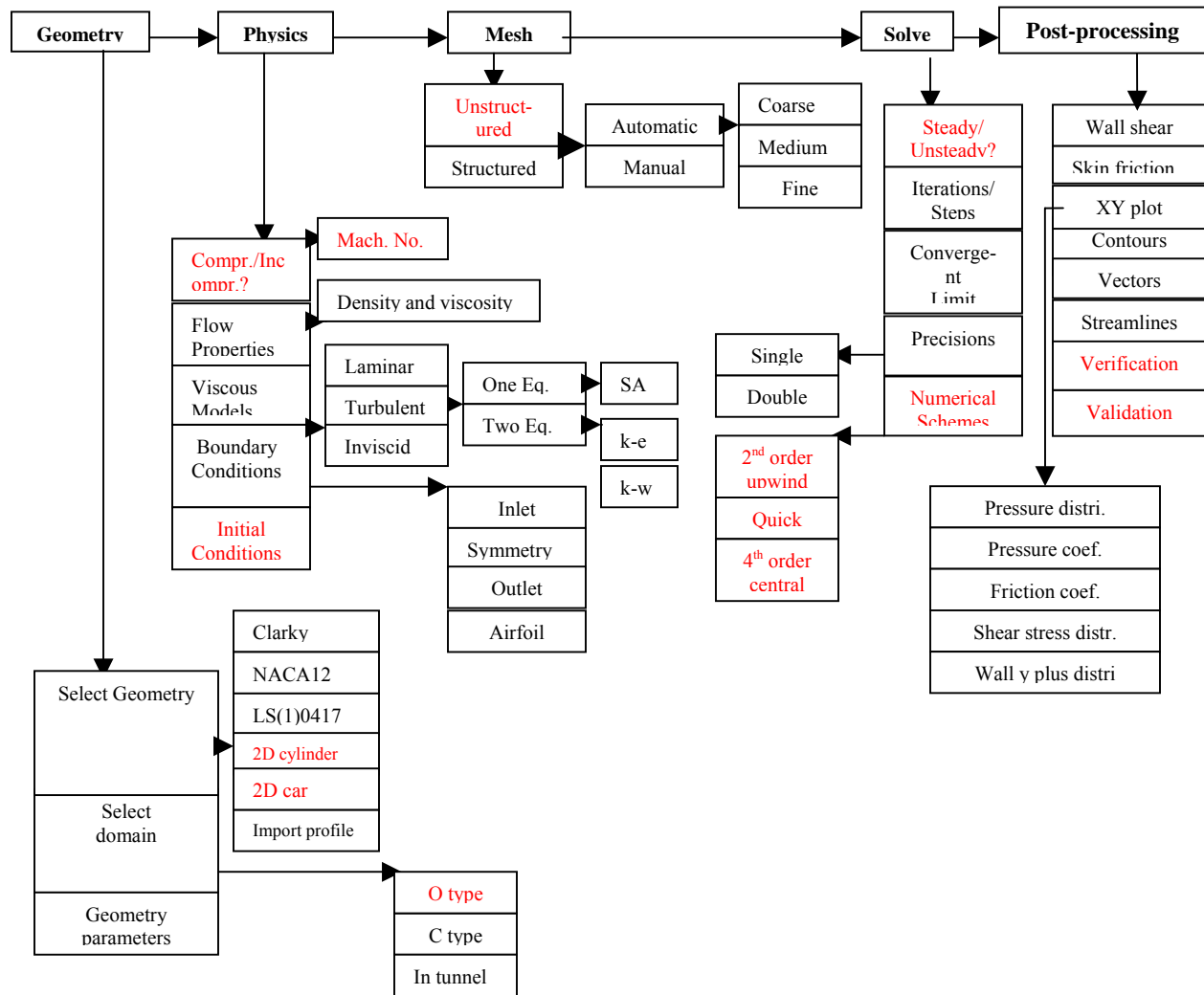


Fig. 11. Flow chart for combined 2D advanced external flow template

Acknowledgements

National Science Foundation Course, Curriculum and Laboratory Improvement - Educational Materials Development Program Award #0126589 under the administration of R. Seals, sponsor project. We would like to thank Prof. Elizabeth Fisher for her input and help in implementing the pipe flow template at Cornell University. IIHR staff member Mark Wilson provided computer support.

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Author Biographies

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ALRIC ROTHMAYER is a professor of aerospace engineering and engineering mechanics with 17 years experience in teaching undergraduate and graduate courses in aerospace engineering. His research interests include viscous flow, computational fluid dynamics, asymptotic methods and boundary layer theory, and aircraft icing.

GANESH RAJAGOPALAN is a professor of aerospace engineering with twenty years of experience in teaching. He has developed a number of undergraduate courses with emphasis on integrating experimental techniques with theory. Dr. Rajagopalan's research emphasis has centered on computationally efficient techniques to study the flow field and operational characteristics of rotating machines such as helicopter rotors.

SHOURYA PRAKASH OTTA is currently a graduate student in Department of Aerospace Engineering. He graduated from Indian Institute of Technology – Kanpur, India with Bachelor of Technology in Aerospace Engineering in 2000. He worked with Matrix CFD Solutions (a subsidiary of ICEM CFD Engineering) in India from 2000 to 2003.

DAVID A. CAUGHEY is a professor in the Sibley School of mechanical and aerospace engineering at Cornell University. He has more than 30 years research experience in developing CFD algorithms, most recently applied to turbulent, reacting flows. He and Professor James A. Liggett co-authored the first interactive text book for introductory fluid mechanics.

RAJESH BHASKARAN is Director of Swanson Engineering Simulation Program in the Sibley School of Mechanical and Aerospace Engineering at Cornell University. He is leading efforts in the Sibley School to integrate contemporary simulation technologies into the mechanical and aerospace engineering curriculum. He received a Ph.D. in Aerospace Engineering from Iowa State University in 1996.

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BARBARA J. HUTCHINGS is currently the Director of Strategic Partnership at Fluent Inc., the leading commercial supplier of CFD software. Barbara joined Fluent at its inception in 1983, after graduating from the Thayer School of Engineering at Dartmouth College with an M.S. degree. She has been working in the field of applied CFD for 20 years and has an active interest in the use of software tools for engineering education.

SHANE MOEYKENS received his Ph.D. in Mechanical Engineering from Iowa State University in 1994. He is the University Program Manager at Fluent Inc. as well as the FlowLab Product Manager.

Invention and Innovation in a Product-Centered Chemical Industry

George Stephanopoulos

Massachusetts Institute of Technology

A WebCAST Lecture

October 26, 2004

Outline

Part-1:

State of and Trends in the Chemical Industry

Part-2:

The Response of the Chemical Companies

Part-3:

From a Process-Centered to
a Product-Centered Chemical Industry

Part-4:

What Is Not and What Is a Product

Part-5:

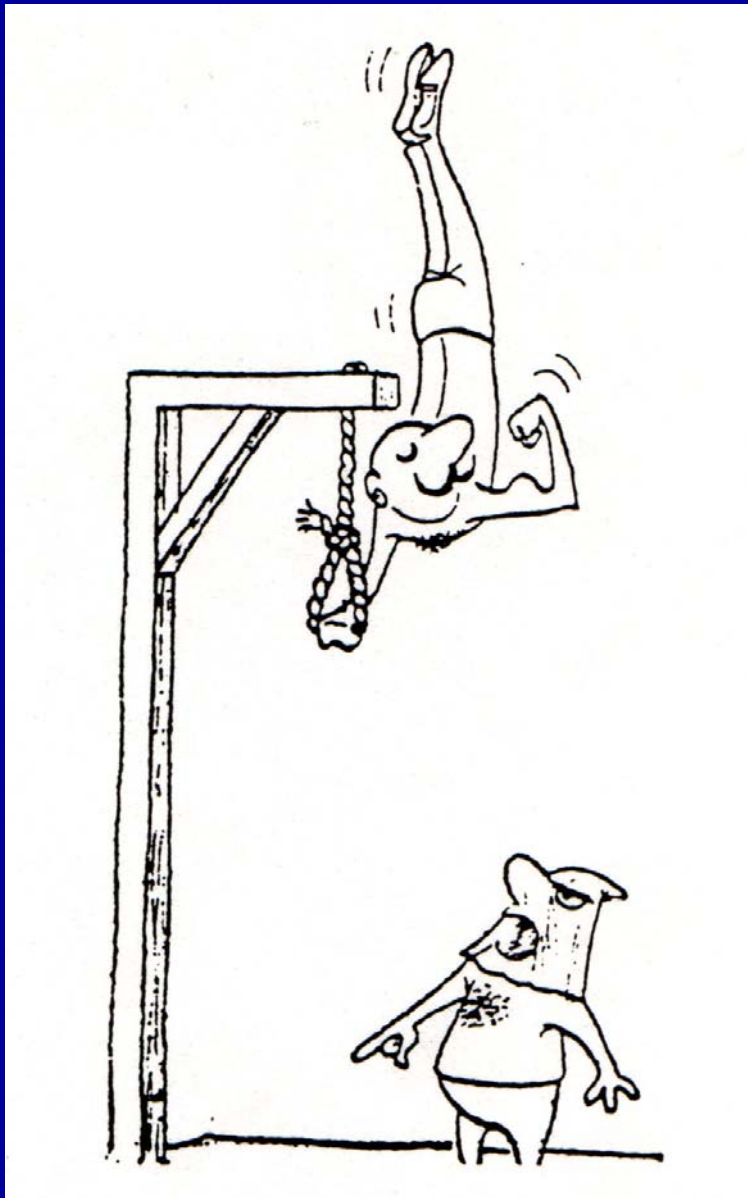
Implications for Industrial R&D

Part-6:

The Challenge for Chemical Engineering Research

Epilogue

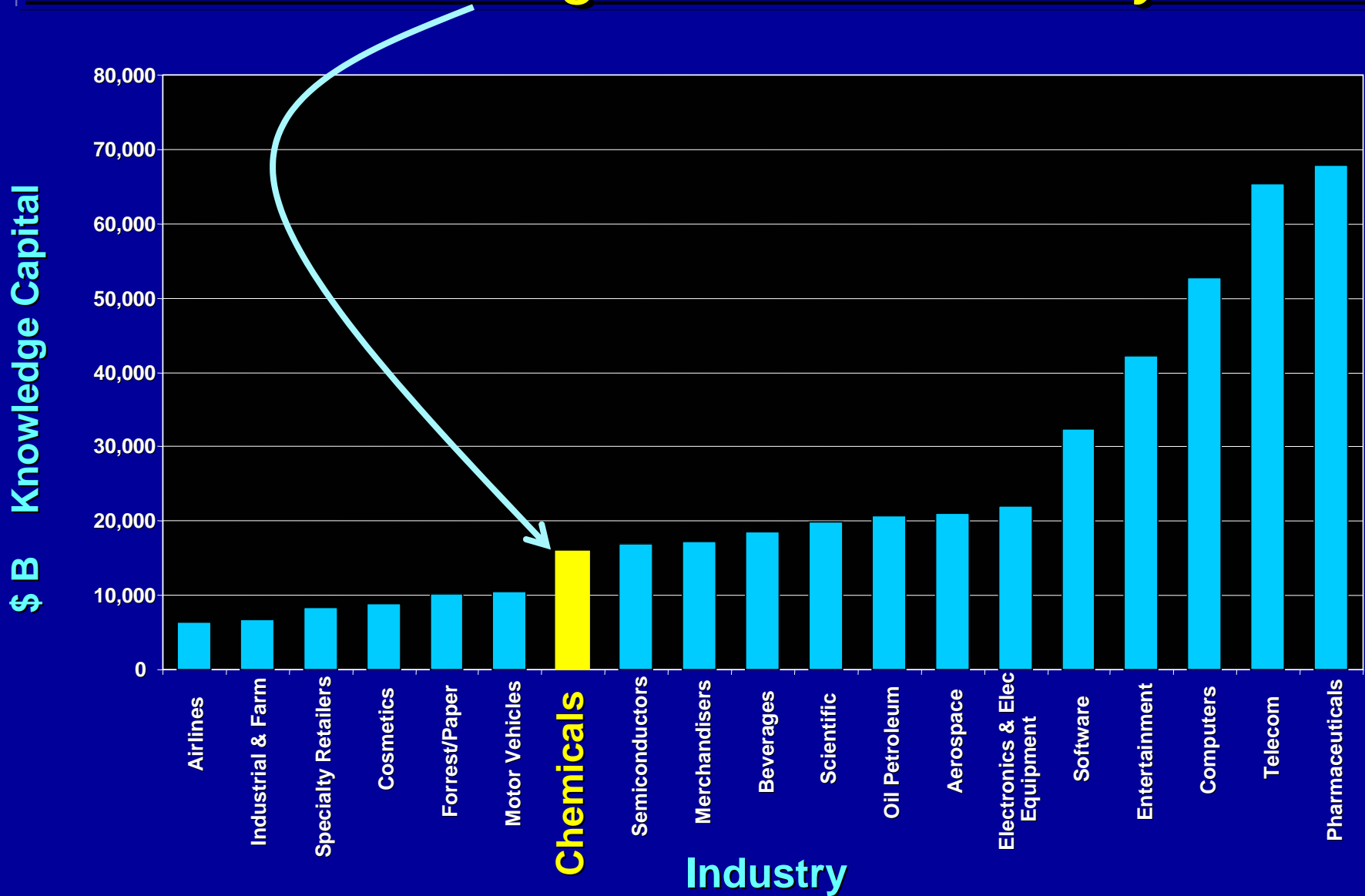
Summary and an Exhortation



Part-1:

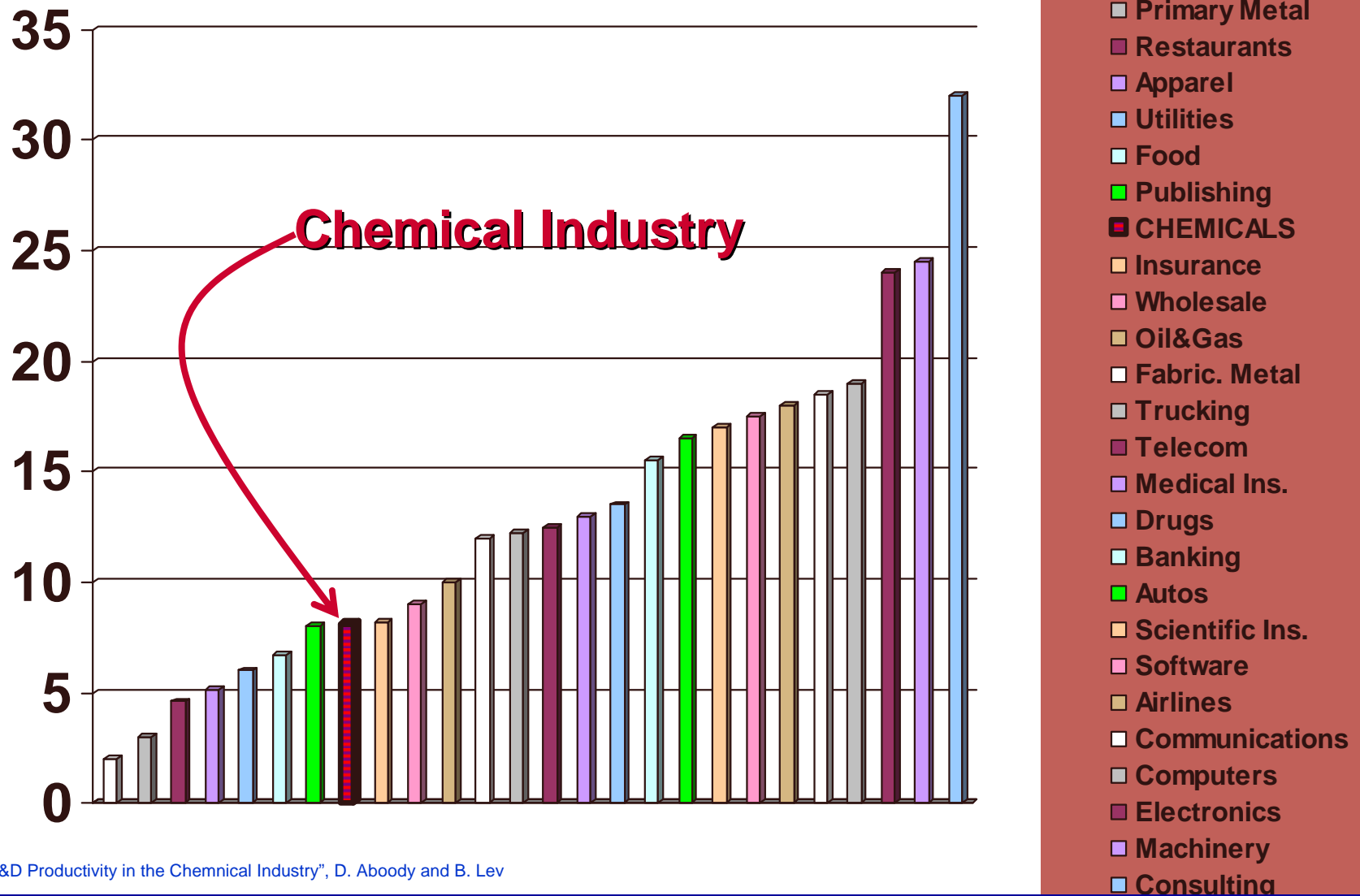
The State of and Trends in the Chemical Industry

Fact-1: Chemical Industry IS NOT Valued as a Knowledge Intensive Industry



Knowledge-Driven Earnings

(average growth rate: 1990-1998)



Fact-2: Productivity in the Chemical Industry Lags Seriously Behind the National Manufacturing Productivity

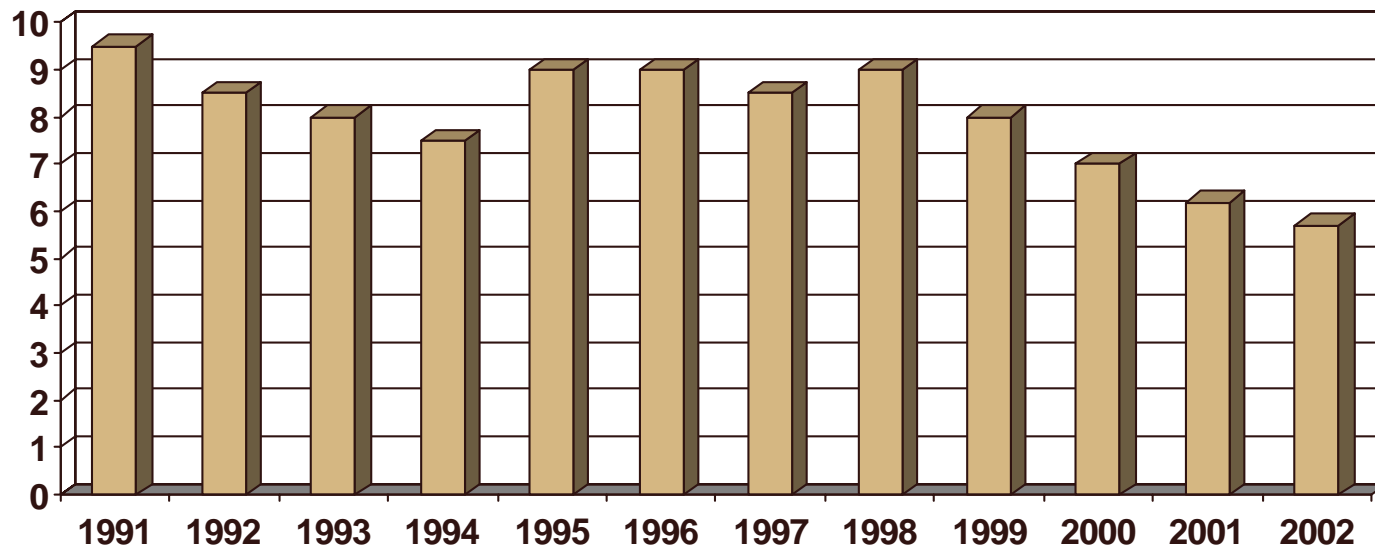
❖ Productivity (output per work hour; 1992=100):

- All Manufacturing :..... 156.8 ('01)
- Chemical industry:..... 123.7 ('01)

Fact-3: Capital Investment has been Sliding

❖ Capital Spending (% of sales):

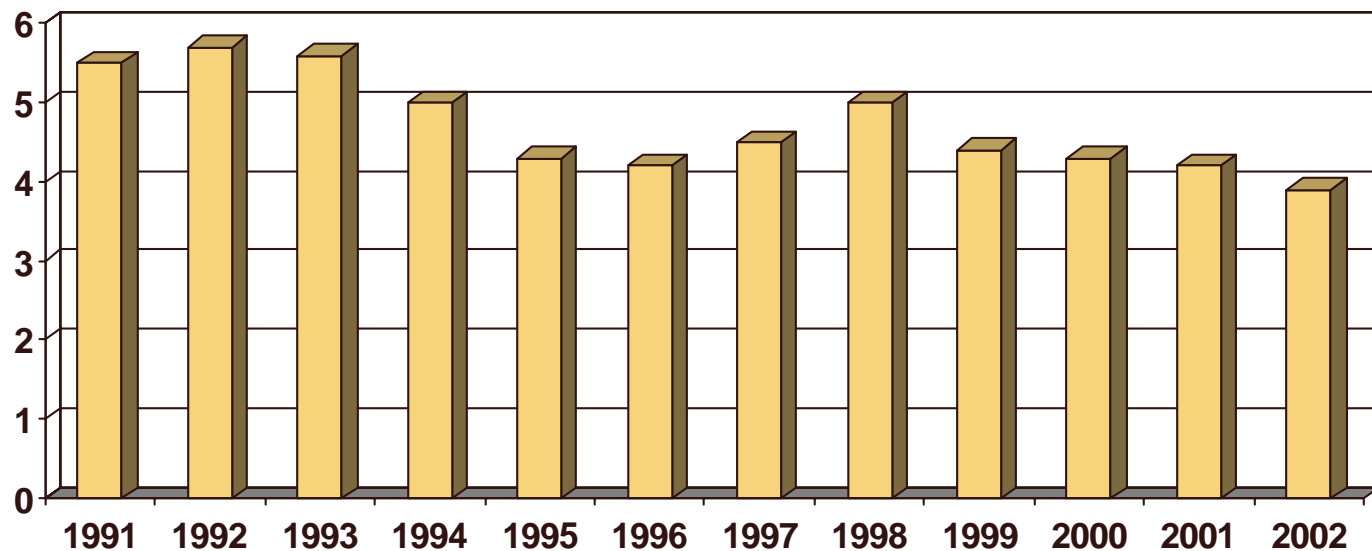
Downward trend



Fact-4: R&D Investment has been Sliding

❖ R&D Investment (% of sales):

❖ Downward trend of total investment

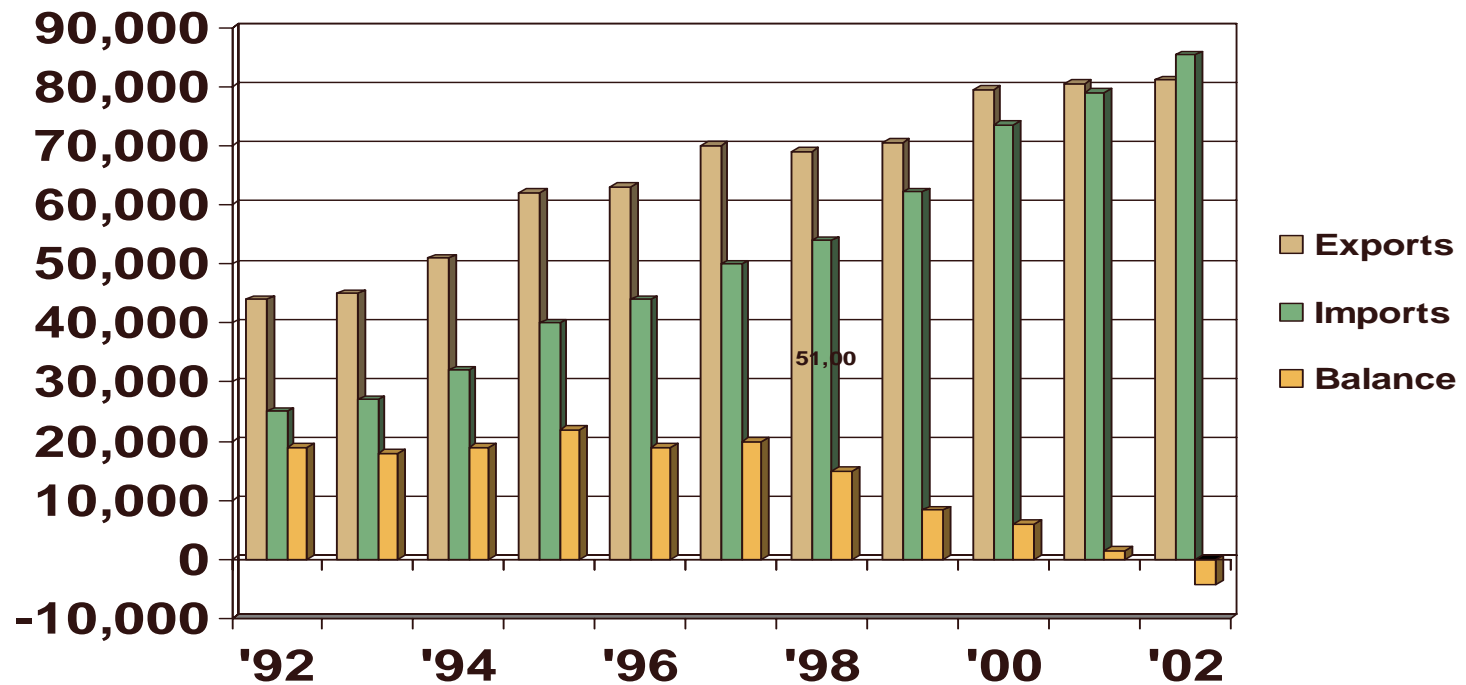


❖ Shift to “Focused”, Business-Unit Based, Product-Process Development Projects

Fact-5: Negative Trade Balance

❖ US Trade Balance:

Deteriorating since 1995. Deficit in 2002 (first time).



Fact-6: Value Growth in Specialties and Products

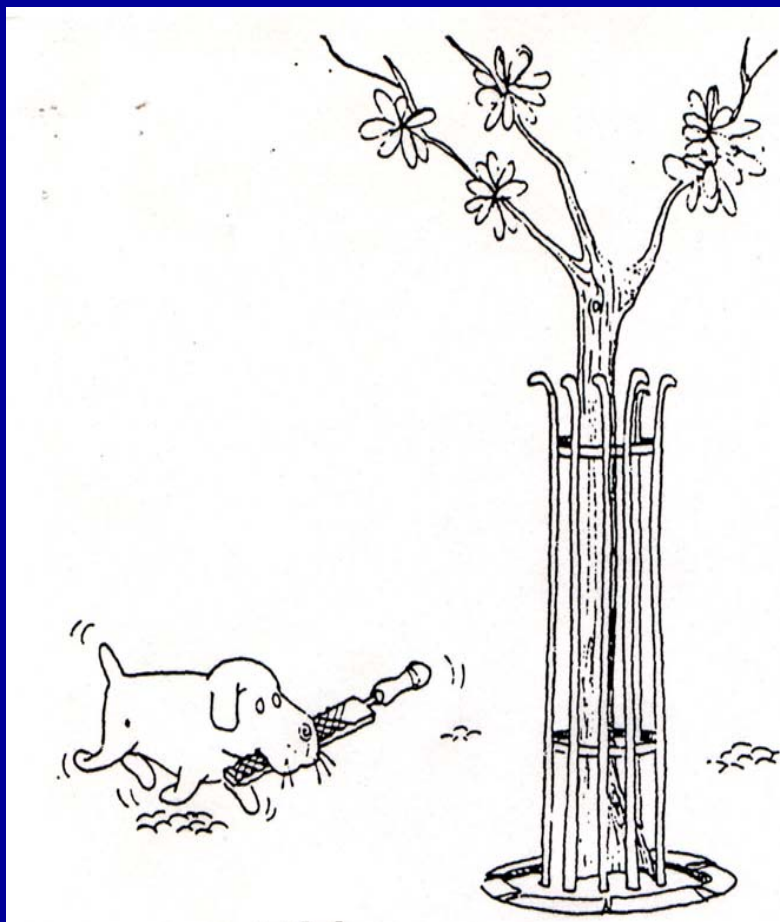
❖ Value: Value growth in specialties and products

- Total chemicals..... 3.5% (annual change)
 - 1991 (318.6 billion \$) 2002 (461.6 billion \$)
- Basic Chemicals..... 1.0%
 - 1991 (142.7 billion \$) 2002 (152.1 billion \$)
- Specialty Chemicals..... 4.6%
 - 1991 (68.6 billion \$) 2002 (107.6 billion \$)
- Life Sciences..... 6.7%
 - 1991 (70.1 billion \$) 2002 (142.0 billion \$)
 - Pharmaceuticals..... 7.1%
 - 1991 (60.3 billion \$) 2002 (128.3 billion \$)
 - Crop Protection..... 3.2%
 - 1991 (9.8 billion \$) 2002 (13.7 billion \$)
- Consumer Products..... 3.8%
 - 1991 (37.2 billion \$) 2002 (51.1 billion \$)

❖ Number of “new molecules” has been decreasing

Recent Trends (1991-2003): Summary

It seems that the Business Model of
the “Diversified” Chemical
company has been seriously
weakened



Part-2:

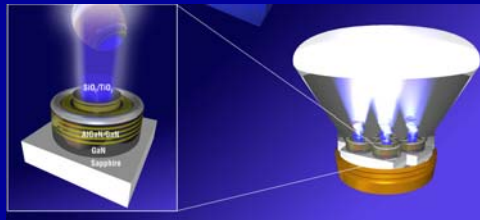
The Response of the Chemical Companies

Element-1: Fractionation of Diversified Chemical Companies

Diversified Chemical Companies



Production-Centric Company



Product-Centric Company



Customer Value-Centric Company

Increasing: Knowledge Content, Value, Economic Return

Element-2: Adjustment of Corporate Management Culture

Production-Centric: Dominate Market Share

Product-Centric: Dominate the Added-Value in a
Product Chain

- Technology-Driven Marketing Culture: Culture of “*Innovation*”

Customer Value-Centric: Dominate the
“Solutions-to-the-Customer”
Channels

Different “Management Cultures” ARE NOT
Commensurable but in CONFLICT with each other

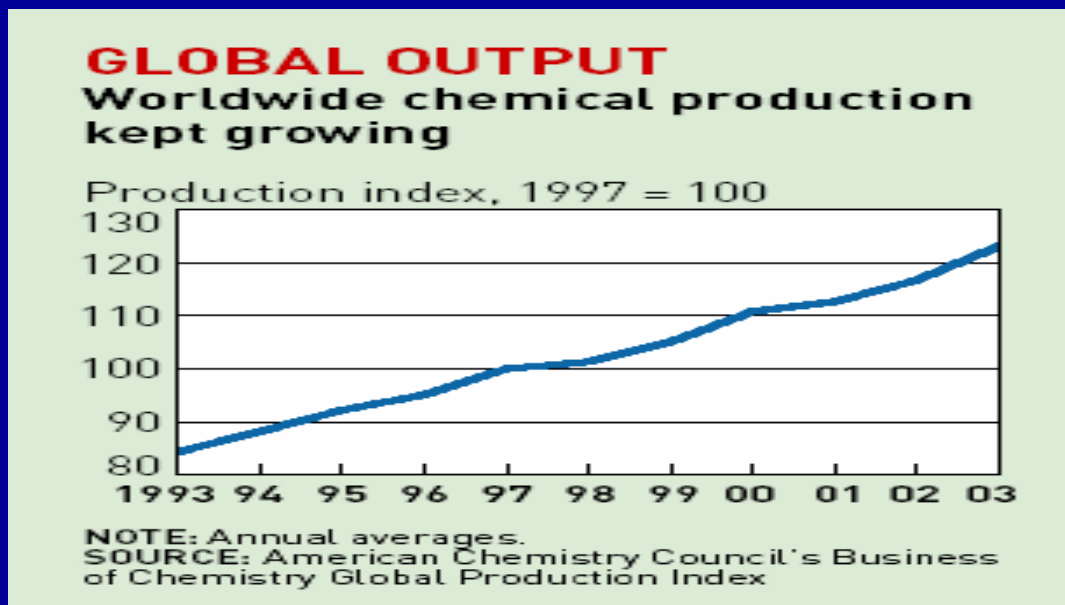
Element-3: *Adjustment in their Global Business Directions*

- ❖ The Demographics of Growth
- ❖ Market Areas of Growth
- ❖ From Process-Centered to Product-Centered Companies

The World Chemical Industry: Growth

1993 – 2003

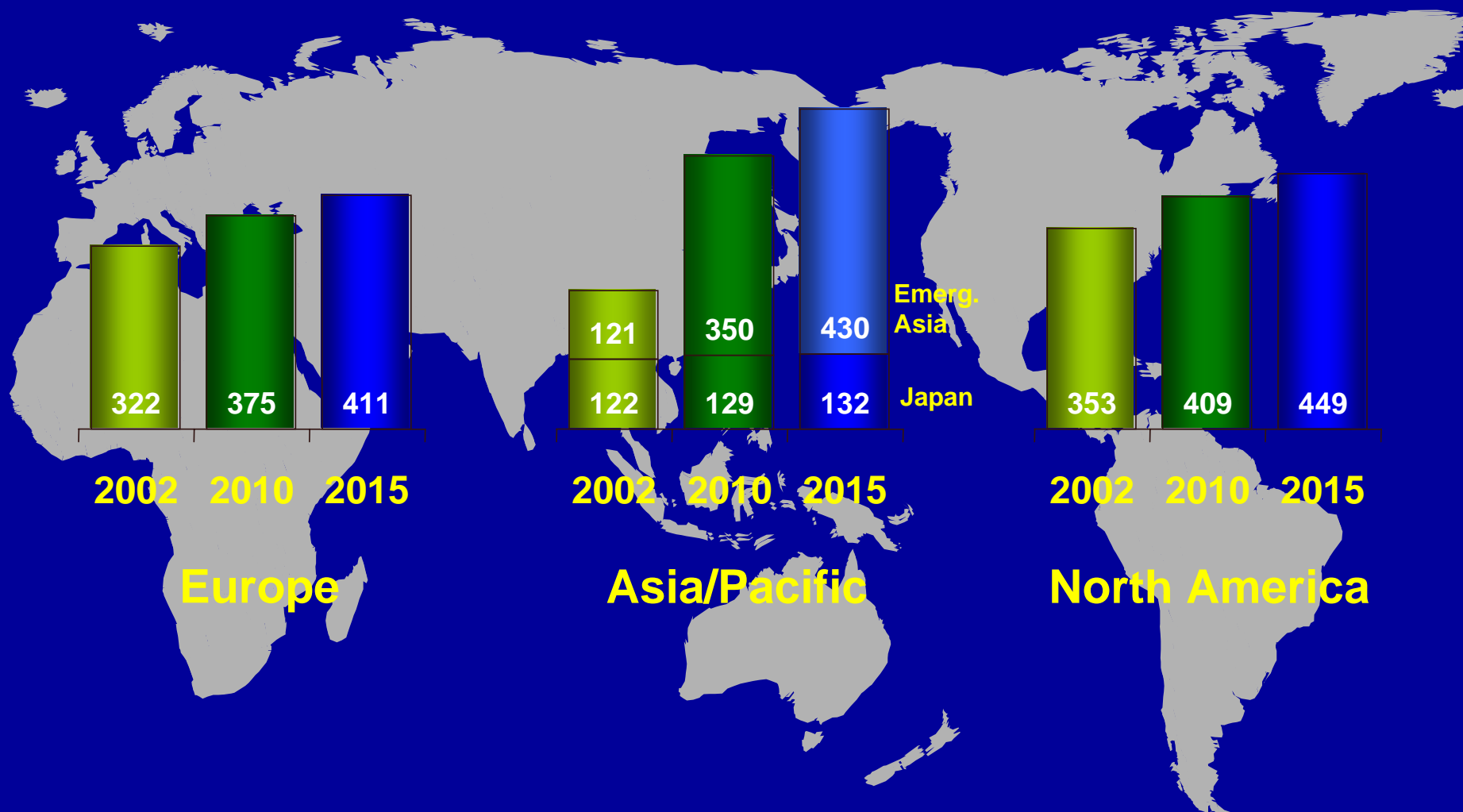
3.9 % per year



2004 – 2015: 2.3 – 2.5 % per year

Below the Gross World Product growth rate:
3.0 – 3.3 %

Chemical Demand by Region 2002 - 2015



Seven (7) Areas for New Business Creation

(METI: Nakagawa Report)

Market Size in 2010: About \$ 2.8 tril

(): Current Size

Info Home Appliances
\$ 160 b (\$ 100 b)

Robots
\$ 16 b (\$ 5 b)

Health, Welfare,
(Devices,
Services)
\$ 700 b (\$ 560 b)

Ecology, Energy,
(Equipment,
Services)
\$ 700 b (\$ 500 b)

Business Support
Services
\$ 1 tr (\$ 700 b)

Fuel Cell
\$ 10 b (Commercialization from Now)

Content (Materials, Fashion, Image, Music)
\$ 130 B (\$ 100 b)

Growing Global Markets of 2010

Size (> \$10 billion), Rate (> 10%)	Size (< \$10 billion), Rate (> 10%)
I&E, Device	
LCD (\$ 90 bil), PDP (\$ 50 bil) Digital Camera (\$20 bil) Cell Phone (\$ 400 bil) Optical Memory (\$ 50 bil)	FED (\$ 2 bil) OLED (\$ 8 bil) Fullerene, Nanotube (\$ 1 bil)
Ecology, Energy	
Amorphous Solar Cell (\$ 30 bil) Lithium Ion Battery (\$ 20 bil)	Biodegradable Polymer (\$ 4.5 bil)
Transportation-related	
Hybrid Car (\$ 13 bil)	Fuel Cell Car (\$ 2.5 bil)
Medical, Security, Welfare	
Home Medical devices/ Systems (\$ 110 bil)	Diagnostics Devices (\$ 4.5 bil)

Where Do the Companies See the Future Growth? (2004-2015)

❖ Commodities:

- Primarily in Asia..... 7-10 % per yr

❖ Product-Oriented Chemicals and Materials:

- “Solutions-to-the-Customer” 10-15% per yr
 - Integration of technological services, chemicals, materials
- Information/Electronics/Telecommunications.....10-15%
 - Semiconductors; Displays; Inks; Specialty polymers; Energy devices
- Medical 6-10 %
 - Diagnostic, Packaging, Fabrics, Surgical supplies
- Safety, Security, Protection 6-10%
 - Diagnostic, Protective Materials
- Life Amenities (Home, Office) 5-8 %
 - Materials/Components for cleaner, healthier environment; Personal care
- Transportation..... 5-7 %
 - Material components and energy devices for automobiles & airplanes

Part-3:

*From a “Process-Centered”
to a
“Product-Centered” Chemical Industry*

“Process-Centered” Company

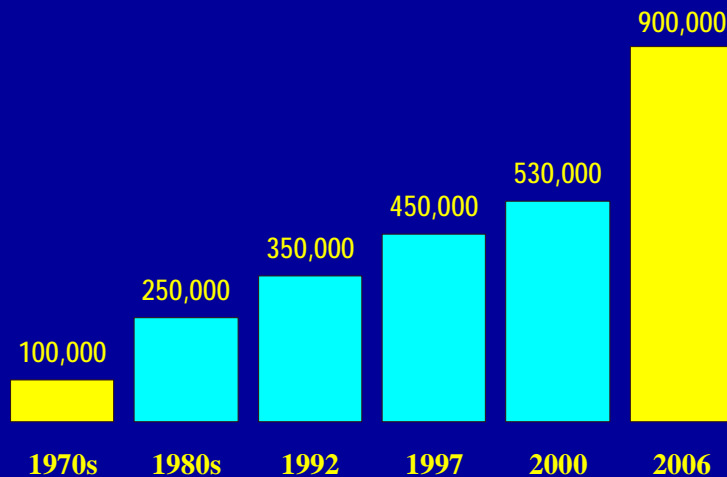
(The Central Dogma of Chemical Engineering)



PROCESS DEVELOPMENT and DESIGN

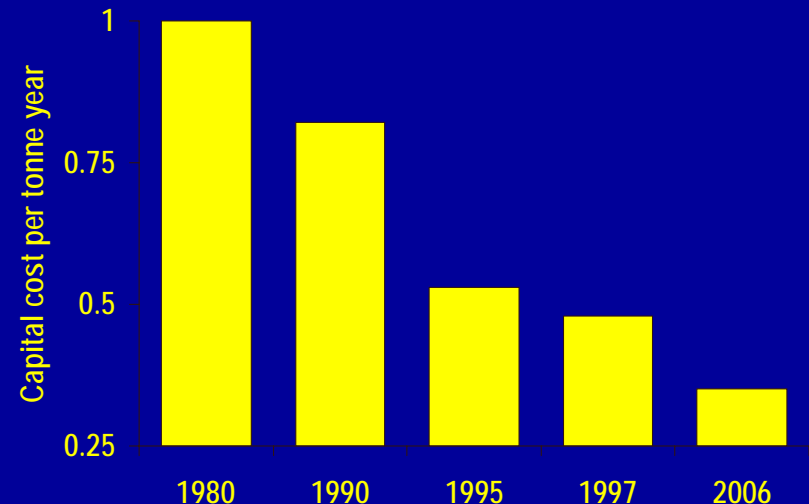
- Select Reaction Pathway(s)
- Design Catalysts; Select Solvents/Diluents/etc.
- Design reactors, separators, and other units
- Synthesize a Cost-Optimal Process with Satisfactory Safety, Operability, and Controllability Characteristics

Testimonial to the Success of “Process Systems Engineering”



PTA Plant Scale

PTA Plant Capital Productivity



Adapted from Jim Trainham

MCC's "Process-Centered" R&D

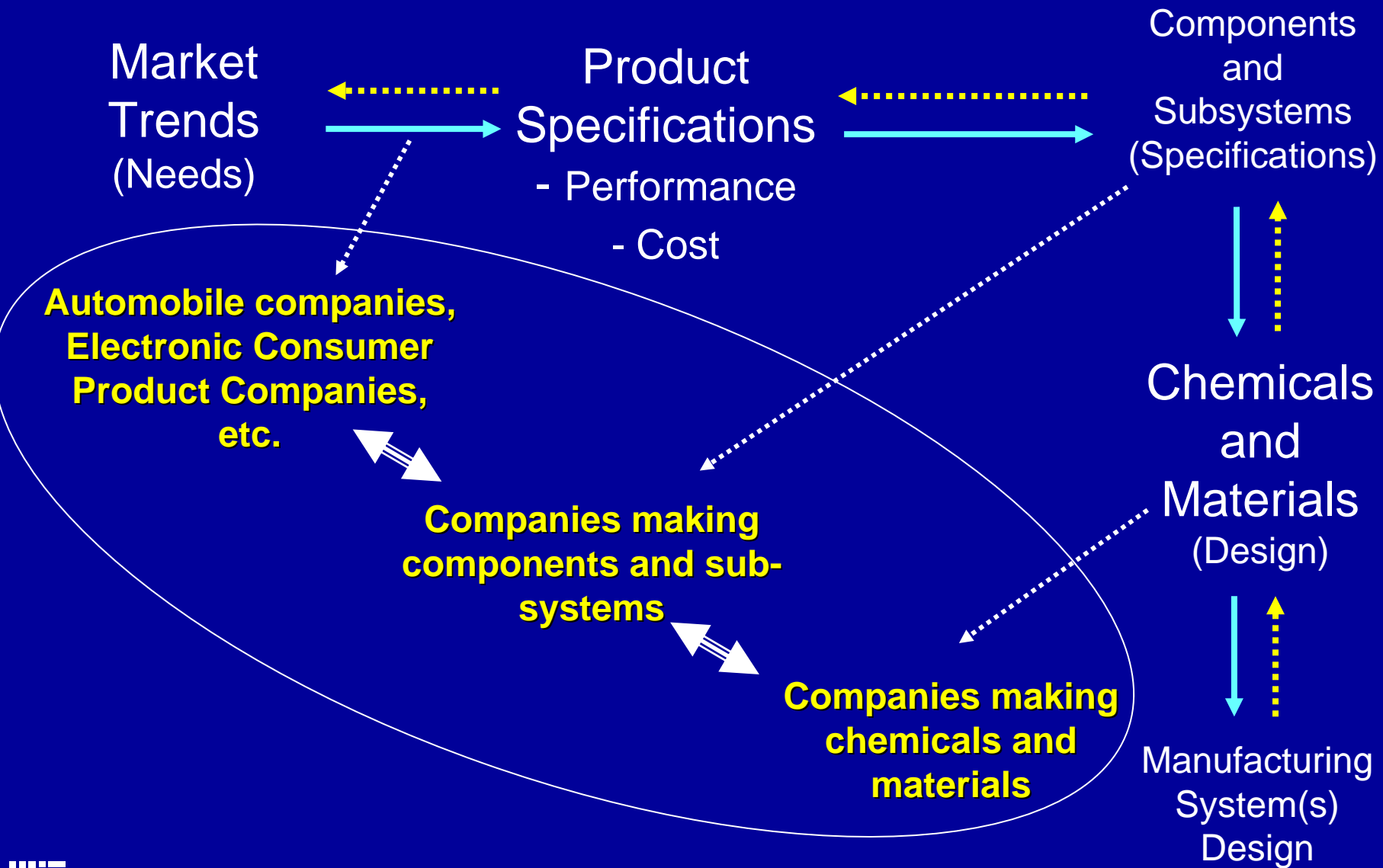
- ❖ Excellent R&D in Catalysis
- ❖ Integrated Process Development
- ❖ World-Class Process Systems Engineering
- ❖ Very effective Process Operations and Business Optimization

Unfortunately these capabilities
are not sufficient to provide today

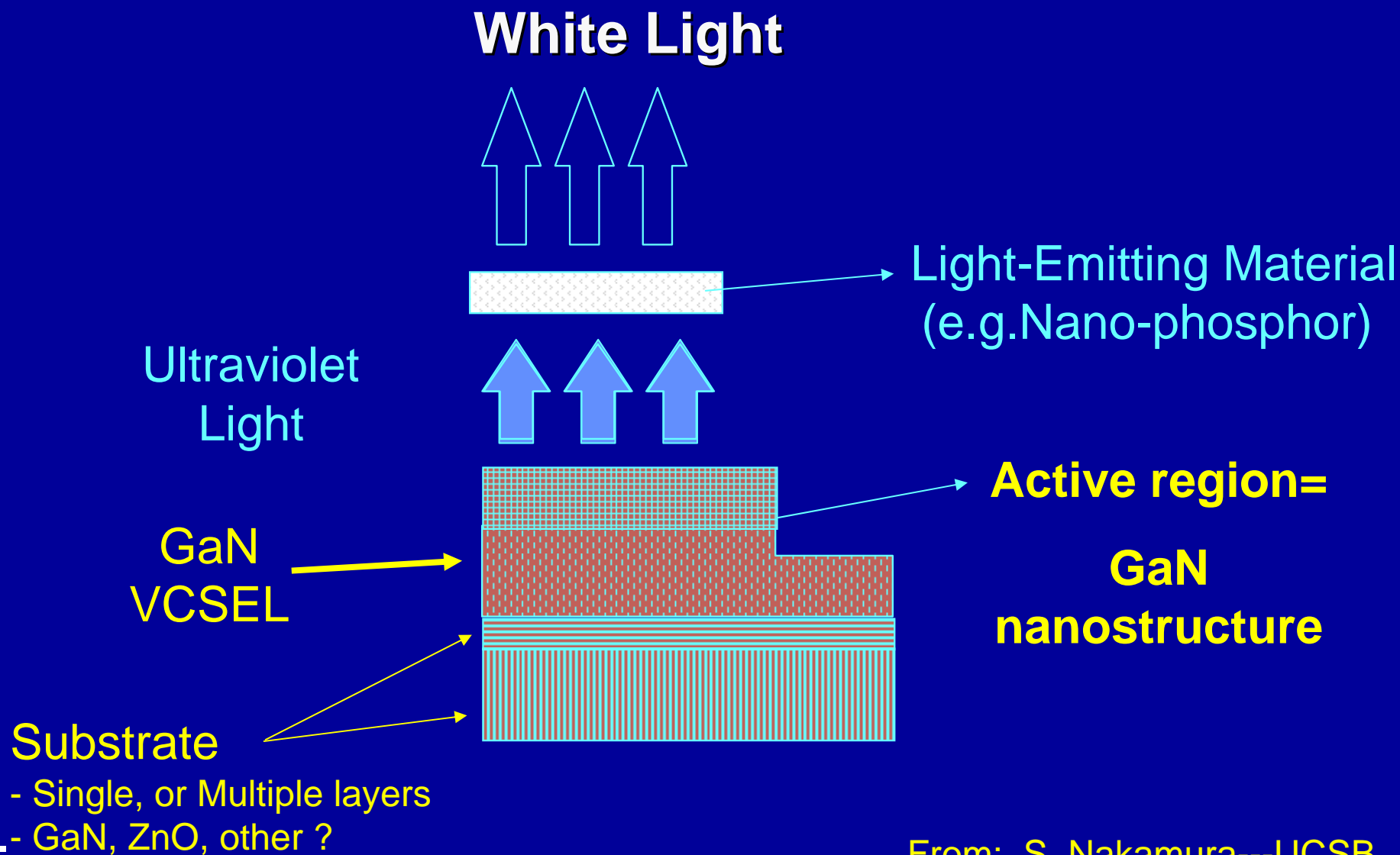
DIFFERENTIATING COMPETITIVENESS

“Product-Centered” Chemical Industry

(The new Dogma for Chemical Engineering)



An Example: Solid-State Lighting and Displays



An Example: Solid-State Lighting and Displays

- ❖ Markets (2010) \$ 9.0 billion
 - Solid-State Lighting\$ 6.5 billion
 - Blue-NUV light emission\$ 1.2
 - Next generation of DVD
 - Automobile lights
 - High-Frequency Devices\$ 0.2
 - Microwave devices for ubiquitous communication
 - Dielectric Scintillator\$ 0.3
 - Dielectric devices; Diagnostic systems
 - Optical Devices \$ 0.5
 - Optical switching
 - Displays
 - Miscellaneous \$ 0.3

An Example: Solid-State Lighting and Displays

❖ Materials

- Substrates for light emitting diodes (LED)
 - UV; Blue/Near UV
- Light emitting materials
 - Organic (small molecules, polymers); Inorganic (phosphors); Hybrids
- Supportive materials
 - Sealants; radical scavengers; etc.

❖ Processes

- Continuous/Batch, Solid-Fluid processes for making the above materials
- Discrete processes for making the devices

An Example: Solid-State Lighting and Displays

❖ “What” Materials to Make ?

- Substrates:
 - GaN, ZnO, other? Single-layer; Multiple layers ?
- Molecular structure and macroscopic morphological structure for
 - light-emitting materials
 - sealants

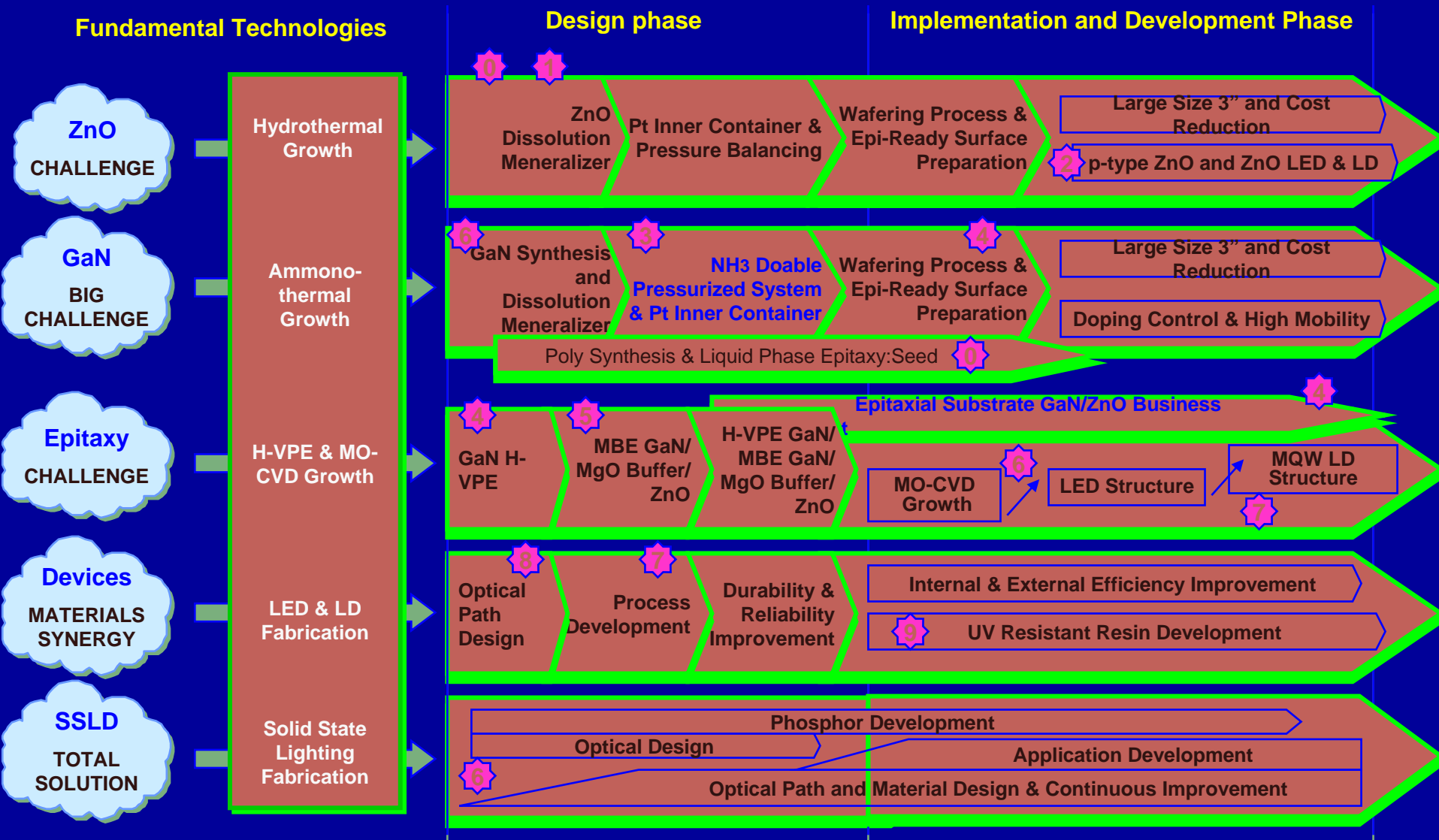
❖ “How” to Make the Materials ?

- GaN and ZnO with very low dislocations' density require technological breakthroughs

❖ Design of the LED devices for high-extraction

❖ Manufacturing the component elements

An Example: Solid-State Lighting and Displays (Partial Technology Road-Map)



An Example: Solid-State Lighting and Displays

- ❖ Can One Company do Everything? NO
- ❖ How does a chemical company decide whether to address these market needs or not?
- ❖ How does a company decide what business position to take?
 - Materials only; Materials and components;
- ❖ How does a chemical company decide “what” to make, and thus what R&D to undertake?
- ❖ What are the requirements for the success of such an undertaking?

Part-4:

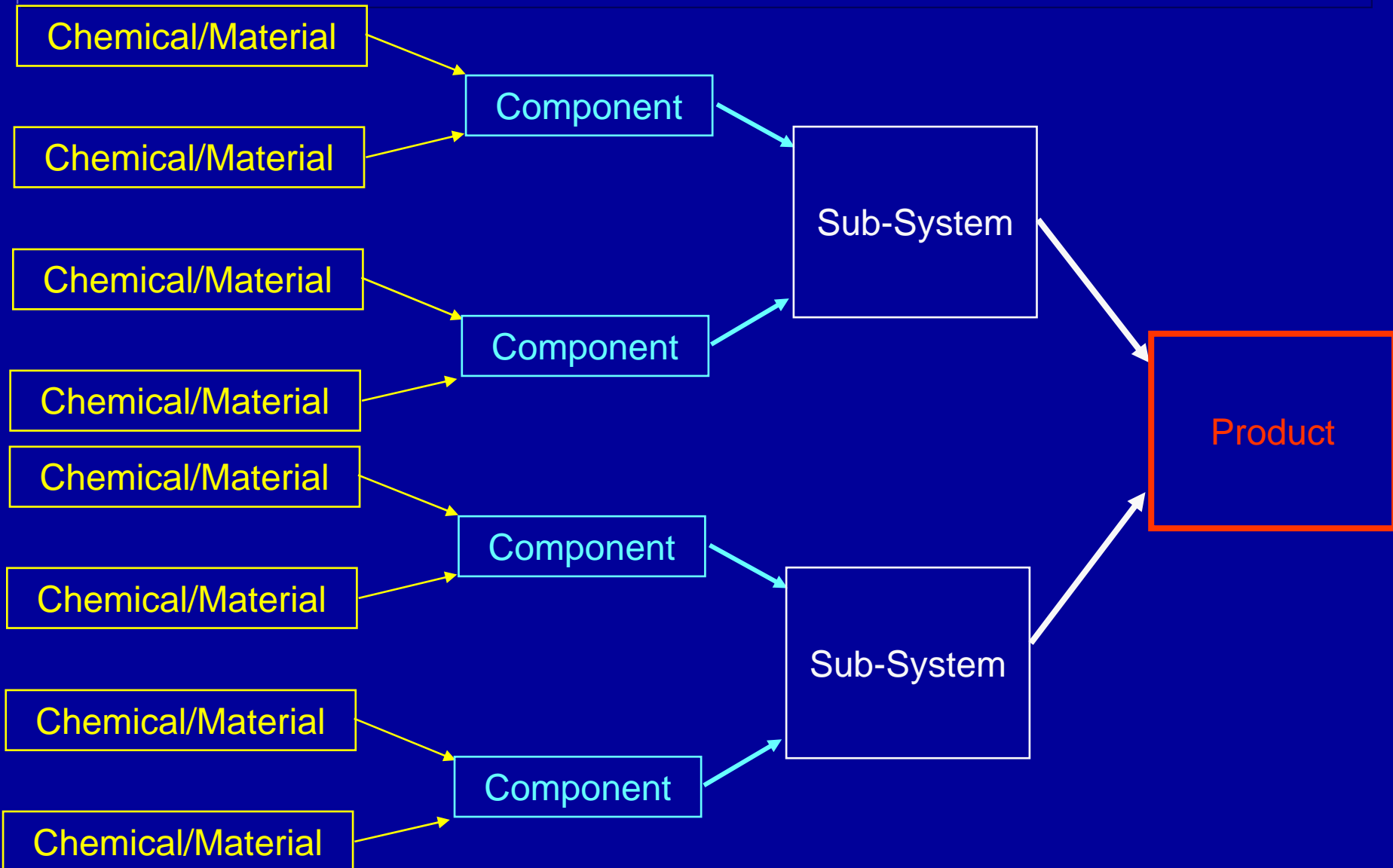
*What Is and What Is Not
Product Design
in a “Product-Centered”
Chemical Company?*

Product Design

- ❖ Is NOT just the design of a Molecule with Desired Properties
- ❖ Is a complicated engineering system
 - With desired functions, and
 - At acceptable cost

The Product Supply-Chain

(Also Defines the Technology Supply-Chain)



What Is Not

- ❖ The design of molecules for improvements in processing efficiencies, e.g.
 - Design of solvents, catalysts, diluents, etc.
- ❖ The design of “new” chemicals and materials intended as commodities, i.e.
 - Not clearly and directly related to specific consumer products

Example: *Design of Pharmaceuticals*

- ❖ A Pharmaceutical is not JUST a molecule, but an integrated design of the
 - Active ingredient molecule(s)
 - Formulation (chemical excipients' composition; physical form)
 - Delivery system

What Is

- Product-Process Development: **Business to Business**
 - Offer improved functionality and substantially reduce the total cost along the Product Supply-Chain, through
 - Product & process forward innovations, and
 - Improved total life-cycle cost
- Product Development: **Business to Consumer**
 - Deliver innovations the consumer values and for which he/she will pay.
 - Deliver functionality that exceeds consumer expectations and challenges their imagination.

Examples: Materials for Displays (Business to Business)

❖ Replacement of Glass Substrates:

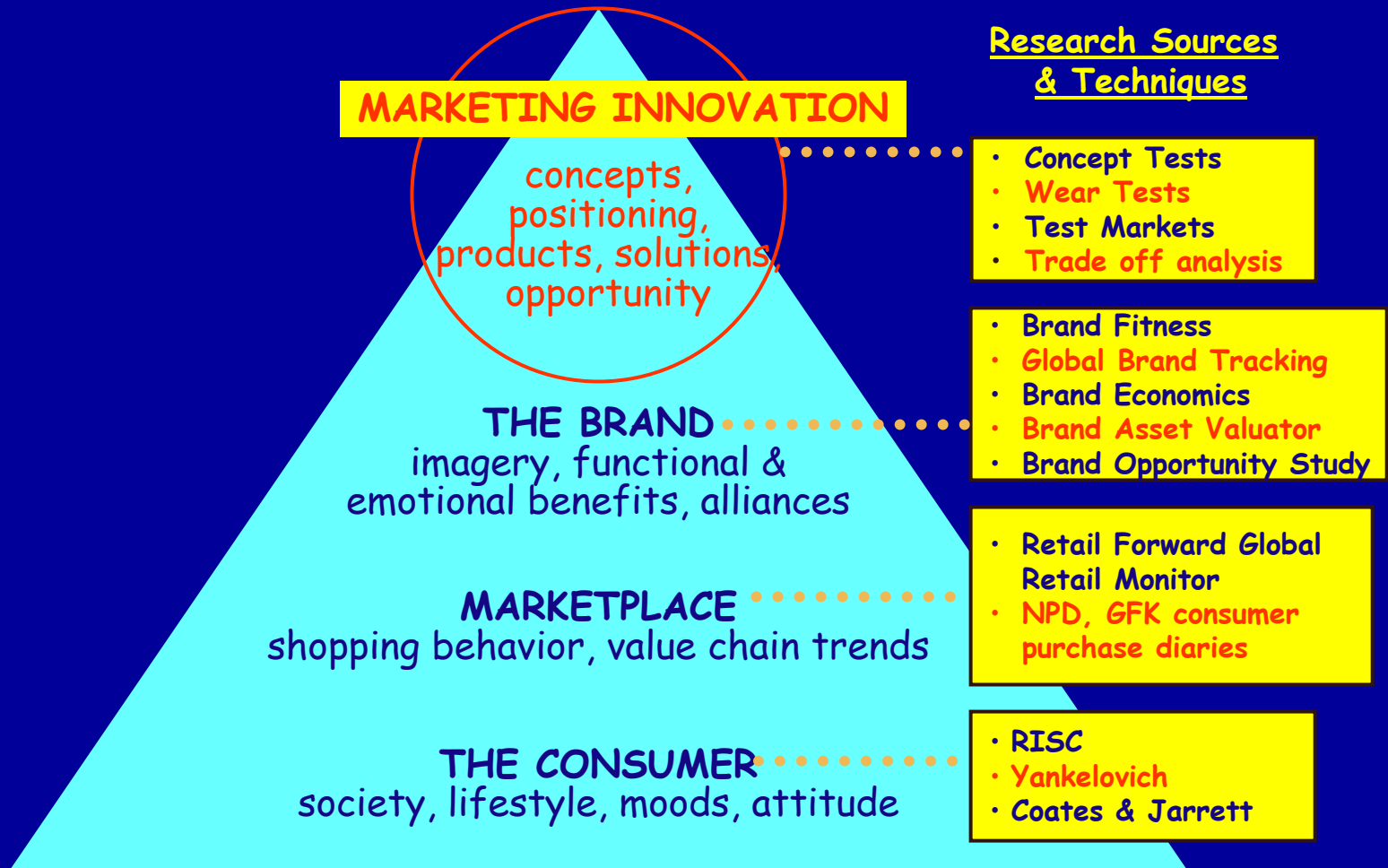
- Consumer products: LCD, PDP, OLED, Paper Display.
 - Transparent, Conductive Polymers with Sufficient Mechanical Integrity, and etc. etc. etc.
 - Different specs for different products
 - Consolidation of films with glass replacement substrate

❖ Materials which consolidate several functions of multi-layered displays

- LCD:
 - Color Filter Film-Polarizing Film-Protection Film
- PDP:
 - EMI Shield Film-IR Absorption Film-Color Control Film-Antireflection Film

❖ Organic Thin Film Transistors (TFT) to replace Si-based films

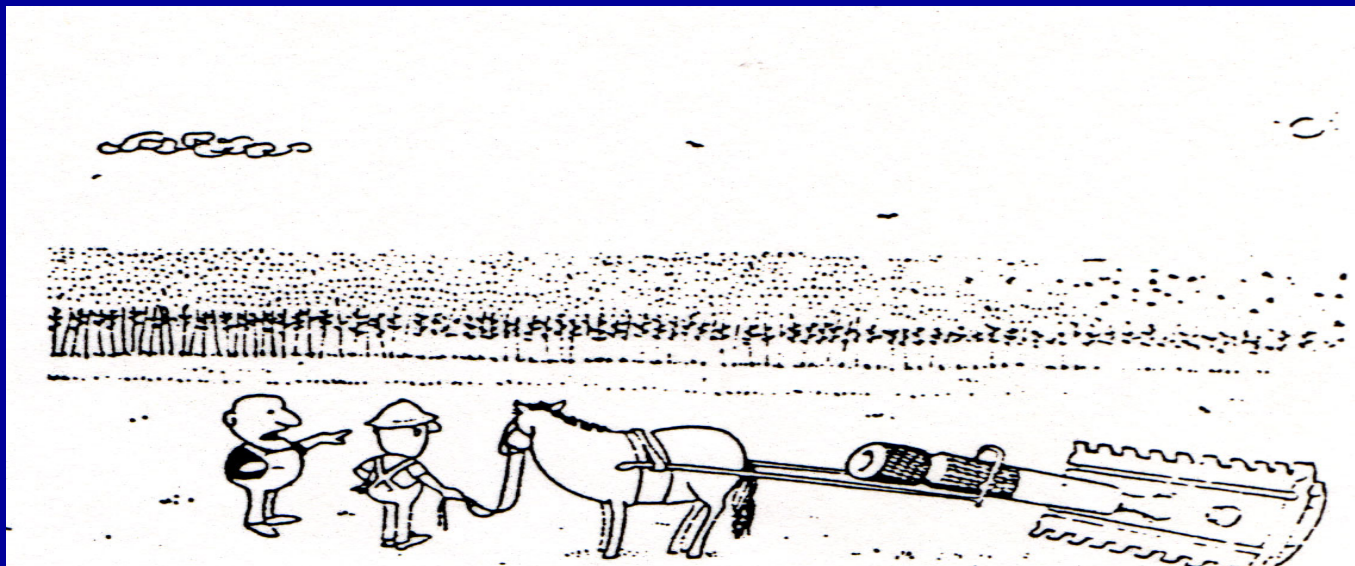
Example: Leather with Lycra (Business to Consumer)



From Jim Trainham

Part-5:

Implications on Industrial R&D from the Shift to a Product-Centered Industry



The Business Model of a “Product-Centered” Chemical Company

- ❖ The Chemicals/Materials will be
 - Targeted for specific Markets and Products
 - Produced in comparatively smaller quantities
- ❖ The Chemicals/Materials must offer Differentiating Value
 - “You cannot make money if you are dealing with the Materials Procurement Department of your customer”
 - Evolutionary improvements in cost and quality is not a differentiating advantage: Everybody does it
 - “You must try to Dominate (be the critical link) in the Product Supply-Chain”
 - **INNOVATION** is the Key

Implications from the Shift

- ❖ **Many More Products than in the past**
 - Smaller Sales Volumes (\$ 10 to \$150 million)
- ❖ **R&TD Investment**
 - High Return.....20-40 % per year
 - Higher Investment..... 6 - 7 % of sales
 - Reduced Life-Cycle of Benefits: Continuous R&D Effort
 - Product-Oriented.....3-4 years
- ❖ **IP Strategy Defines the Technologies to be Developed**
- ❖ **Structure and Culture in the Management of R&D, i.e.**
 - The Culture of “Entrepreneurship”:
 - New Applications
 - New Markets
 - The spirit of the Venture start-up

The Need for Innovation: A Desperate Call from Industry

“Innovation”:

The first successful Commercialization of
an Invention

Innovation

- ❖ Is a Knowledge-Intensive Process
- ❖ Is a Business Activity
- ❖ Is much more than Discovery or Invention
- ❖ Focus on Execution

The Culture of Innovation

DIRECTION

1. A Different and Ambitious Corporate Vision
2. Alignment of Business and R&D Visions and Strategies
3. Integration of Marketing and R&D
 - IP Strategy and Business Positioning
 - The Role of the “Customer”

SPEED

4. Leveraging of Corporate Knowledge and Assets
 - Alliances with other Corporations
 - Alliances with Universities and National Laboratories
5. An Effective and Ambitious R&D Organization
 - Flat Management Structure
 - Ambitious and Entrepreneurial Management Philosophy
 - A Results-Oriented Mindset
6. Rich and Effective Technology Platforms
 - Integrated Technology Platforms as “Engines” of Business Growth

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1. *The New Vision*

Reformation (Product & Services Oriented)

Mitsubishi Chemical Corporation will become a
Dynamic, and Global

- ❖ *Product-Innovator, and*
- ❖ *The Preferred Solutions-Partner*

Rejuvenation (Ambition-Driven Strategy)

Corporate R&TD Aims at the Development of New
Businesses in which MCC can be a Dominant
Player, World-Wide

The Culture of Innovation

DIRECTION

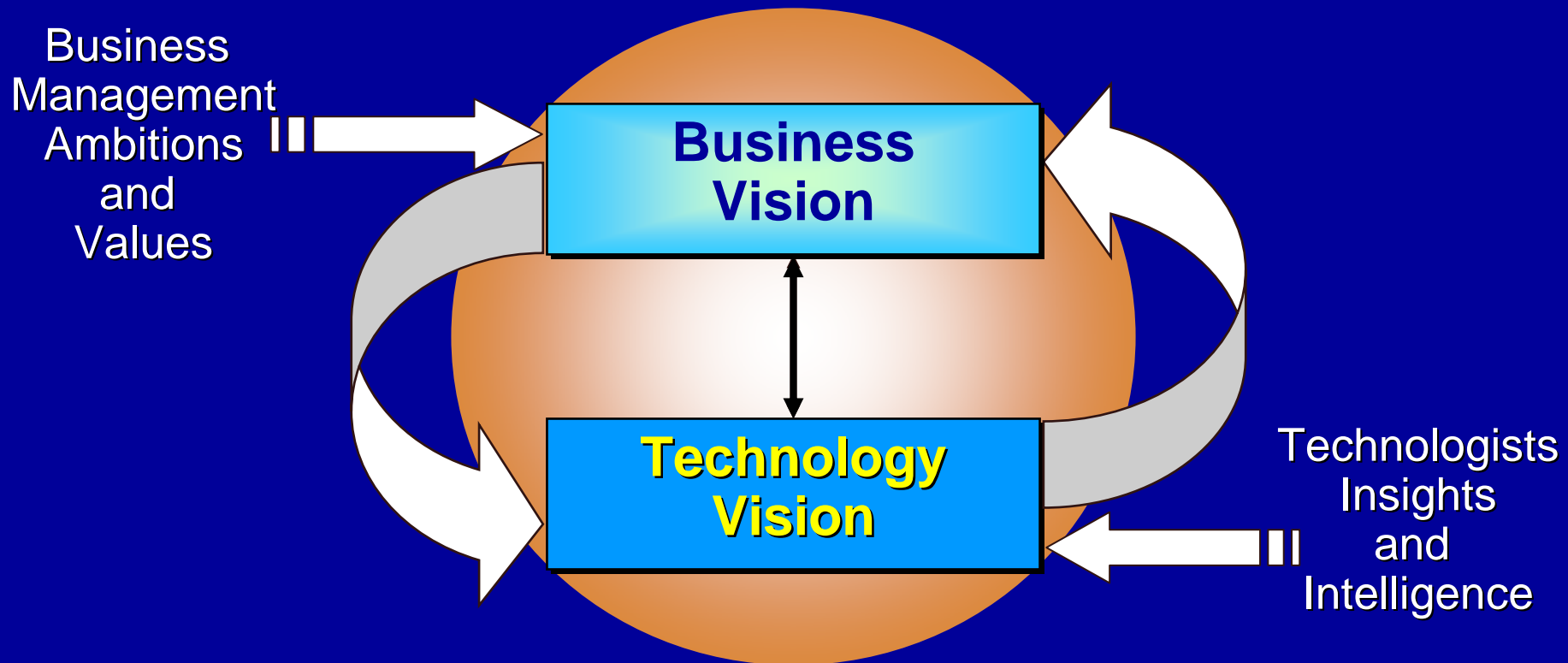
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2. Align Business and R&D Vision and Strategies

Business Vision drives the Technology Vision: 60%



Technology Vision drives the Business Vision: 40%

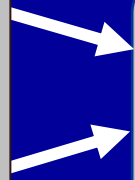
Road-Maps: Linking Technology to Business

Business Vision

CUSTOMER NEEDS
roadmap



**GROWTH MARKETS
&
PRODUCTS**
roadmap



PRODUCTS VISION
(a) cost-performance
(b) Functionality specs
roadmap

PRODUCTS
roadmap

PROCESS
roadmap

**Business
Planning**

Technology Vision

TECHNOLOGY
roadmap
(internal/external)



**TECHNOLOGY
PLATFORMS**
roadmap



R&D PROJECTS
roadmap

**Technology
Planning**



The Culture of Innovation

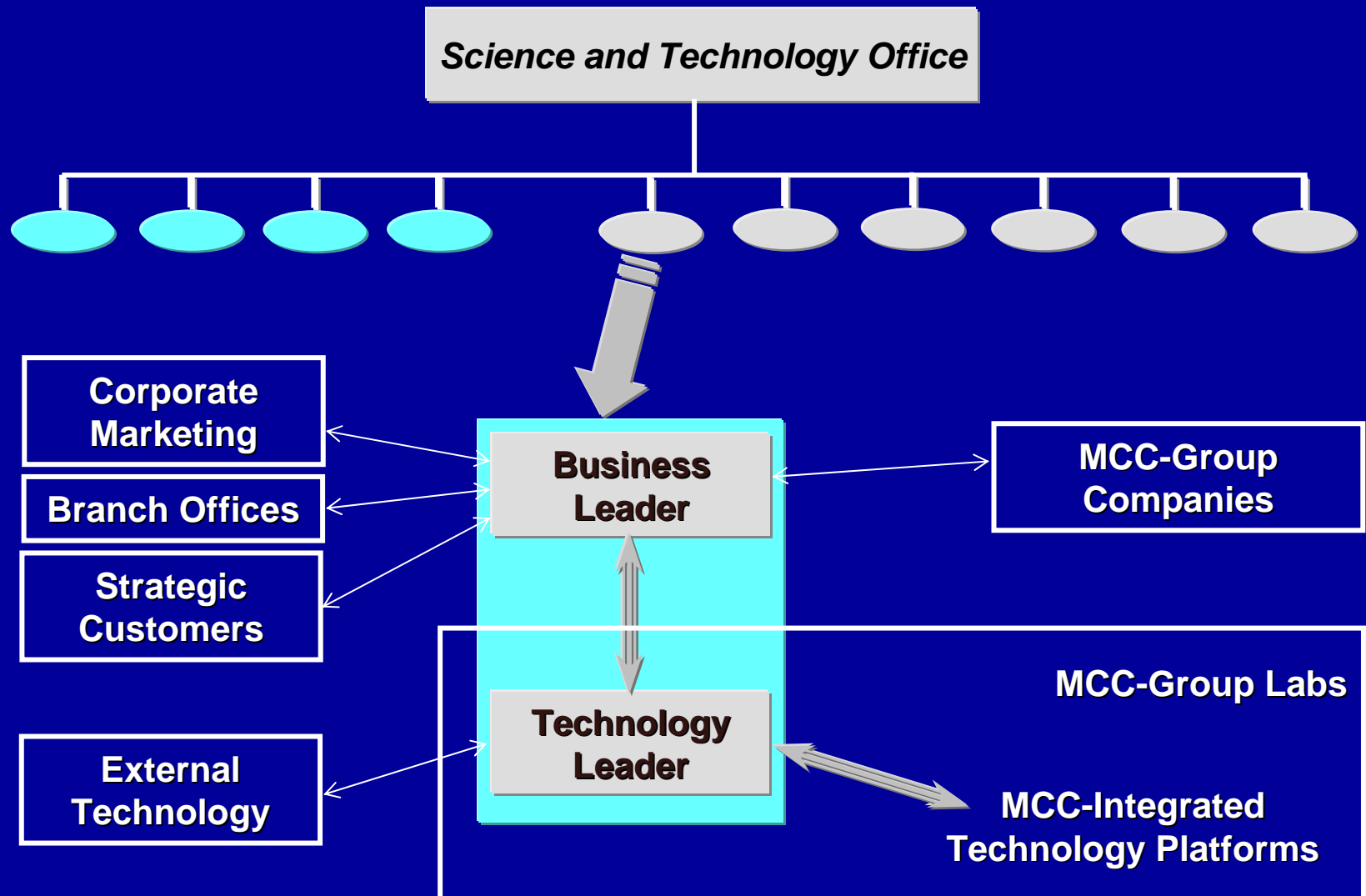
DIRECTION

1. A Different and Ambitious Corporate Vision
2. Alignment of Business and R&D Visions and Strategies
3. **Integration of Marketing and R&D**
 - IP Strategy and Business Positioning
 - The Role of the “Customer”

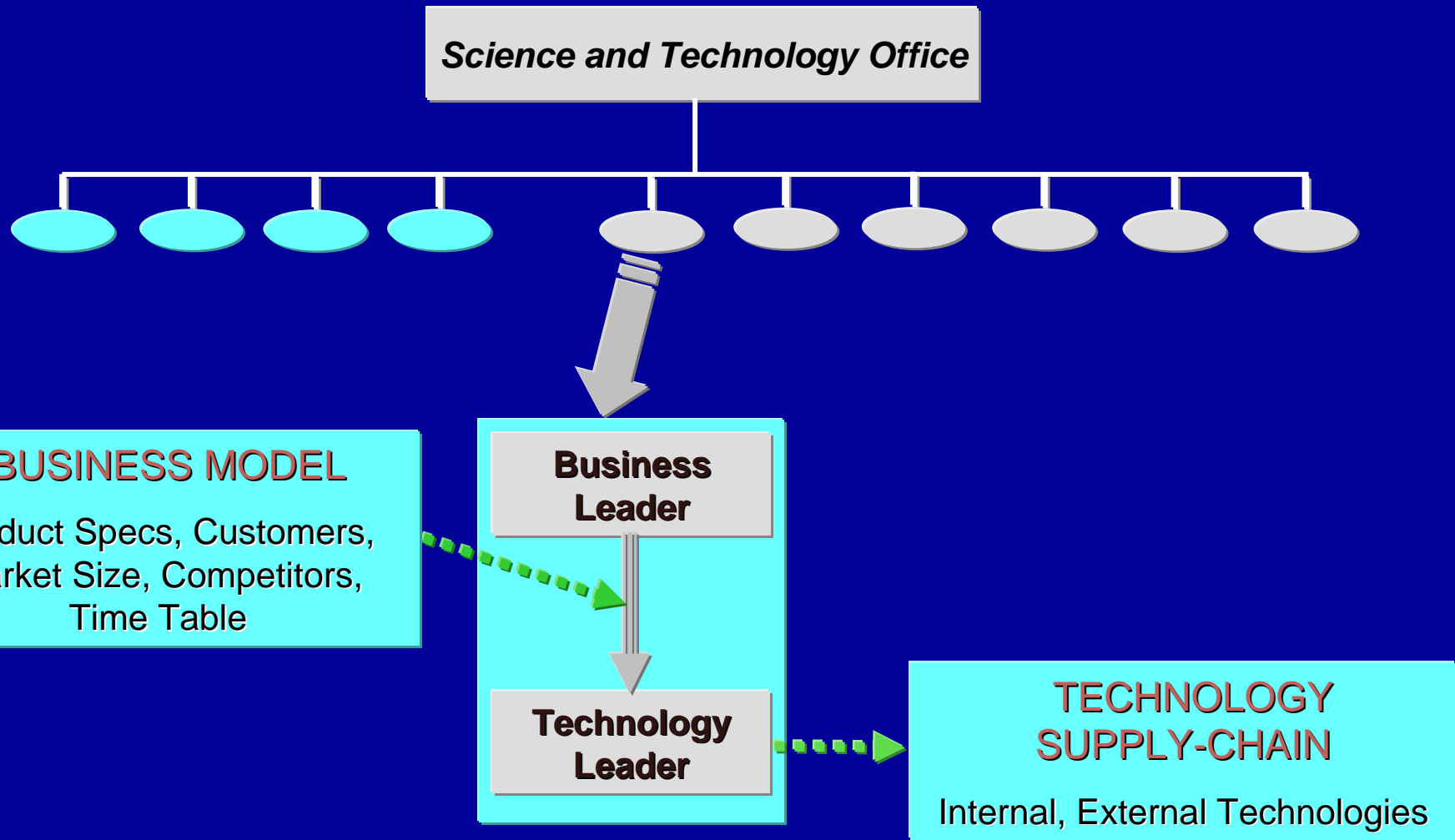
SPEED

4. Leveraging of Corporate Knowledge and Assets
 - Alliances with other Corporations
 - Alliances with Universities and National Laboratories
5. An Effective and Ambitious R&D Organization
 - Flat Management Structure
 - Ambitious and Entrepreneurial Management Philosophy
 - A Results-Oriented Mindset
6. Rich and Effective Technology Platforms
 - Integrated Technology Platforms as “Engines” of Business Growth

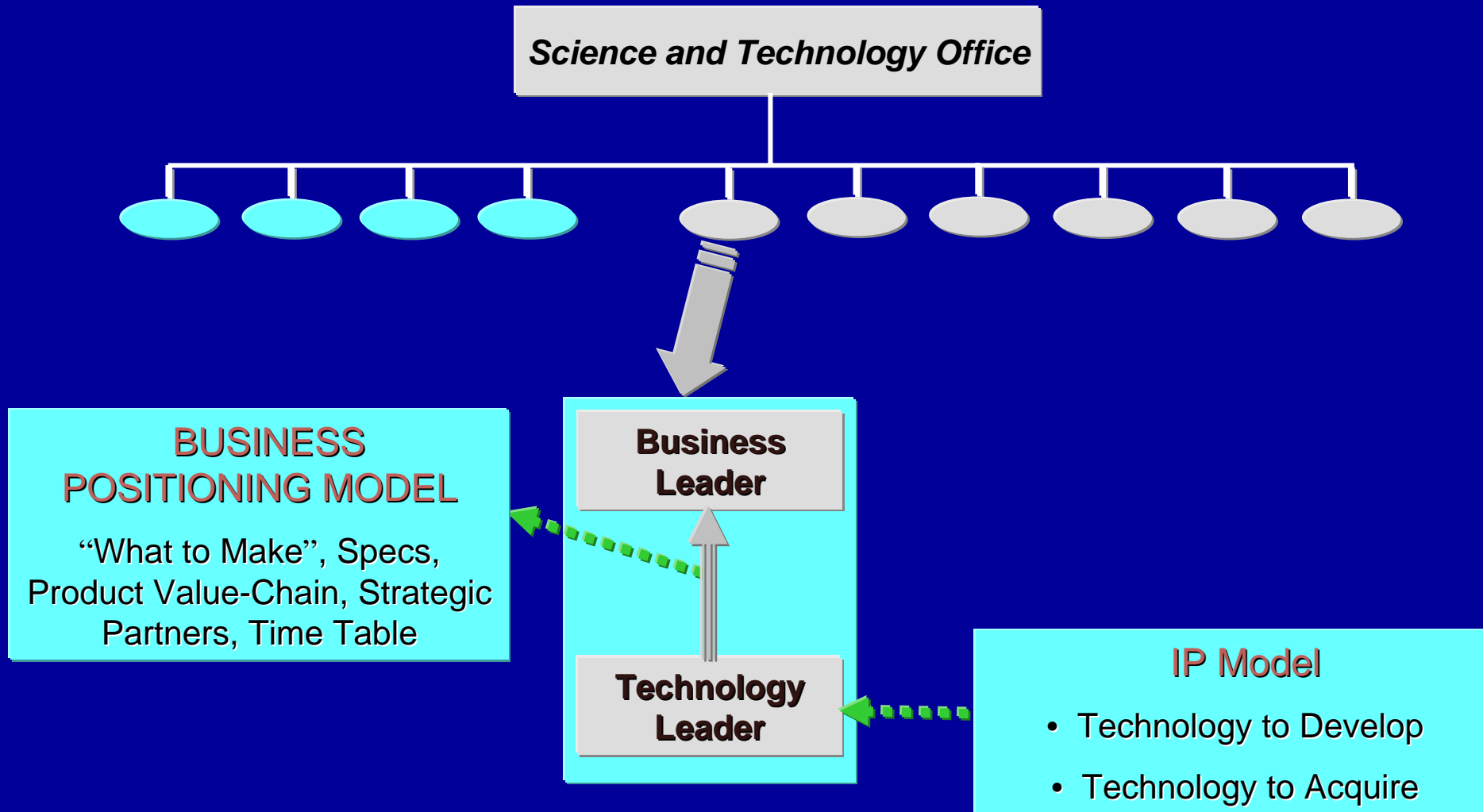
3. *Integration of Marketing and R&D* (Creating Small Entrepreneurial Groups)



3. Integration of Marketing and R&D: (Phase-1: Develop the Technology Supply-Chain)



3. *Integration of Marketing and R&D:* (Phase-2: *Develop the Business Positioning Model*)



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4. *Leveraging Corporate Knowledge and Assets*

- ❖ Exploratory Research in a Product-Centered Chemical Company is Inherently Very Risky, Costly
 - Explosion of New Scientific and Technological Developments
 - Inter-disciplinarity of High-Added Value Technological Platforms
 - Most of the New Ideas come from outside
 - Tackling all possibilities is “Economic Suicide”
 - Universities, National Labs, and Venture Start-Ups are natural partners
- ❖ Product-Development requires collaboration of interacting corporate partners in the Product-Chain
 - Strategic Alliances with Corporate Partners

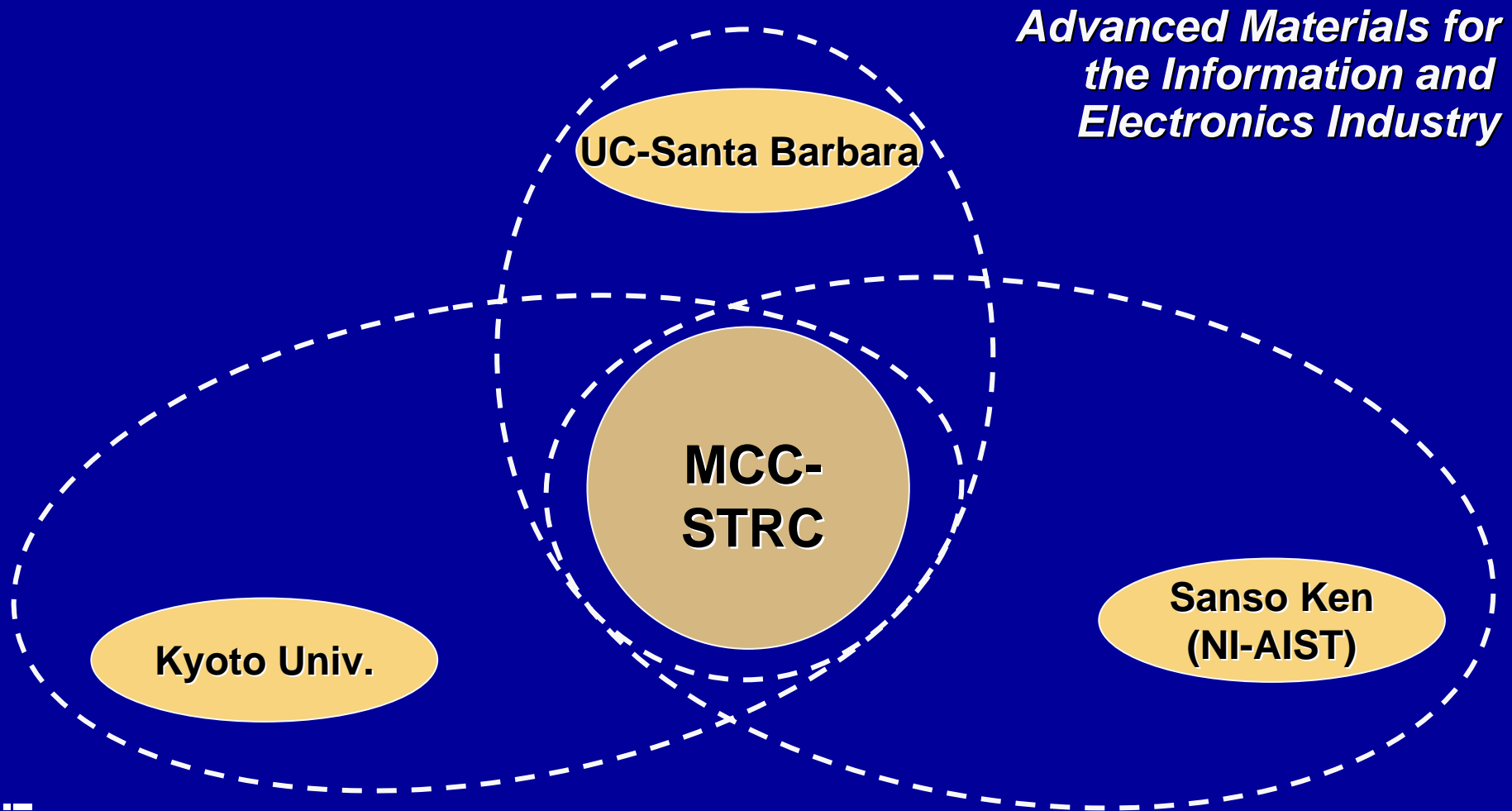
4. Leveraging Corporate Knowledge and Assets (Examples)

Corporate Alliances

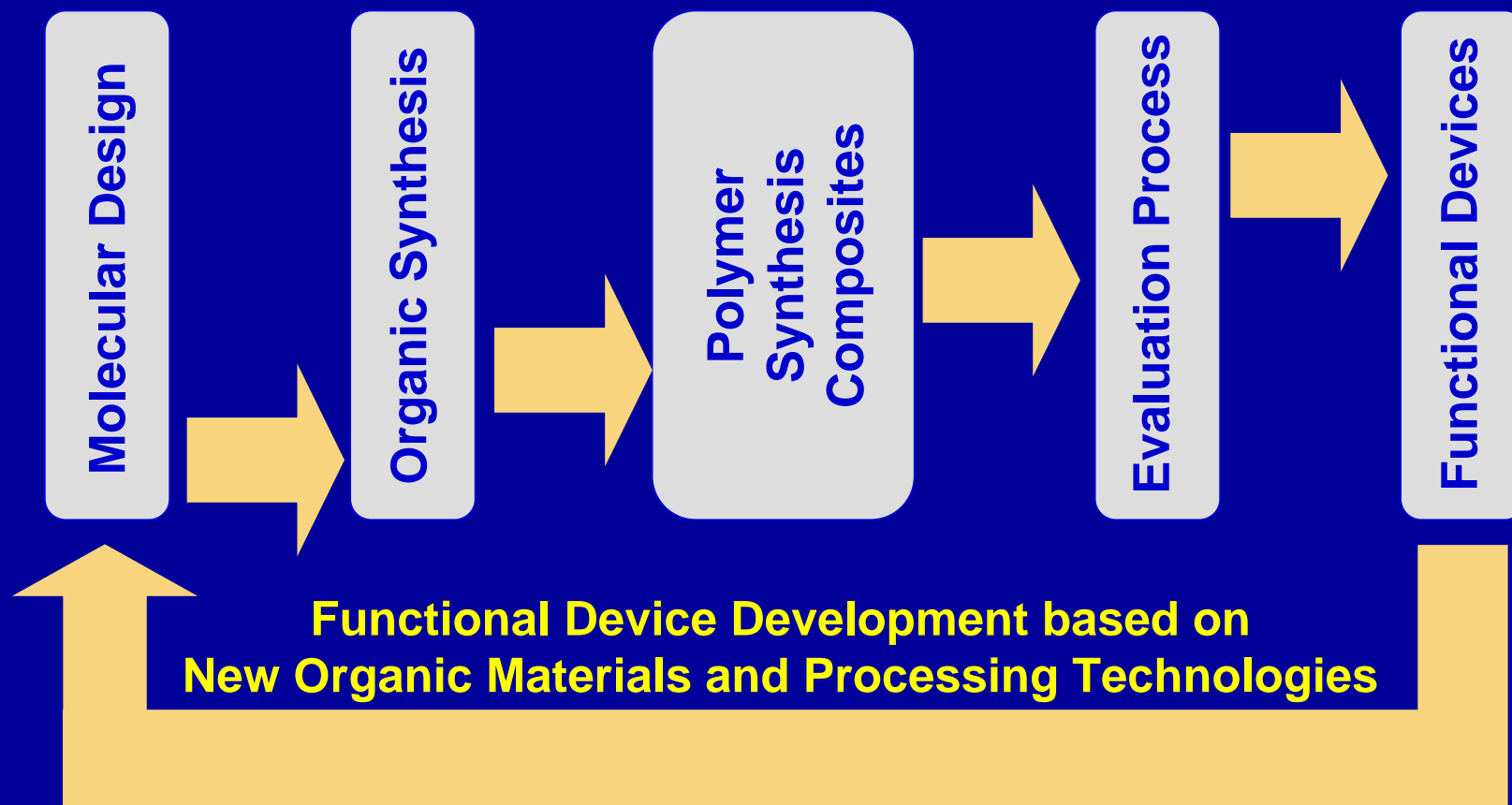
- ❖ Ajinomoto: Biodegradable Polymers from Biomass
- ❖ Corporations X, Y, Z: Solid-State Lighting & Displays
- ❖ Corporations A, B: Materials for automobiles
- ❖ NTT, Hitachi, Rohm, Pioneer: Materials for the electronic and telecommunications devices
- ❖ 30 Corporations: Devices from Nano-Carbon Materials
- ❖ Corporations K,L: Materials and Fabrications for Diagnostic Devices
- ❖ Corporations I,J: Proteomics/Glycomics-based pharmaceuticals

4. Leveraging Corporate Knowledge and Assets (Examples)

Academic Alliances



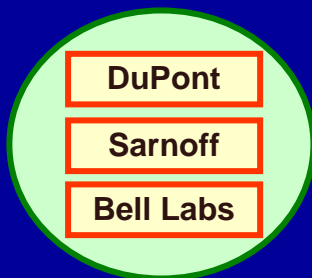
Cross-Company, Cross-Market Segment Vertical Integration at the Kyoto University Alliance



Corporate Alliances: OTFT

Organic TFT on Plastic Substrate (11/10/2002 Announce)

Advanced Technology Program, NIST (National Institute of Standards and Technology)
3 Years. DuPont expects to establish and commercialize for an OLED application by 2007.



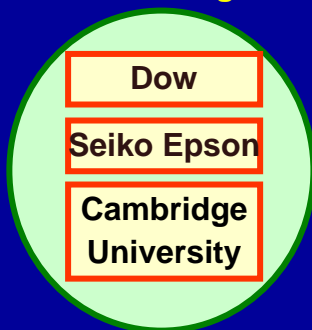
OLED, Flexible Substrate, Cost Effective Printing, OTFT

Active Matrix TFT Design, Video Display Systems

New Material, Design Process

Plastic Logics Inc.(a spin-out from Cambridge University's Cavendish Laboratory)

Organic transistor production by inkjet printing.



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“What Do We Want to Become ? ”



The Culture of Innovation

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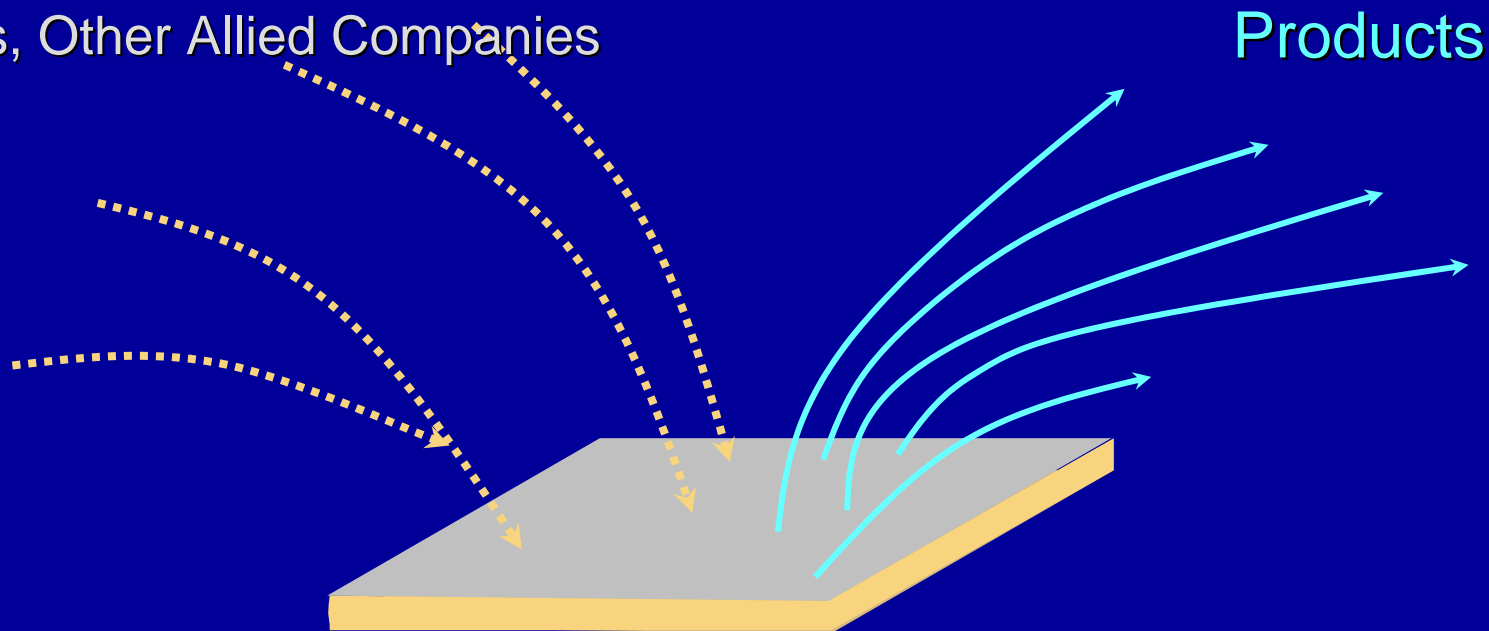
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Integrated Technology Platforms: (Engines of Business Development)

Technologies

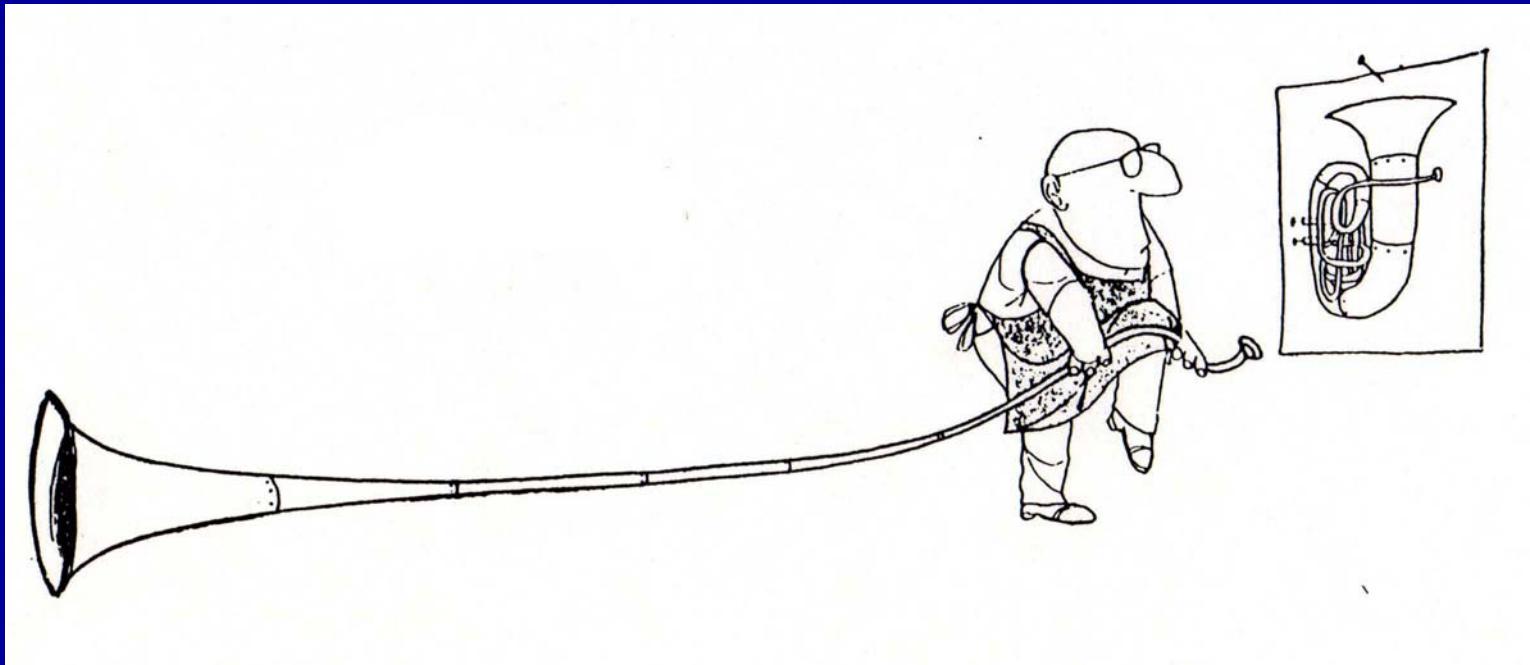
- Internal
- External:
Universities, National Institutes,
Start-Ups, Other Allied Companies



Technology Platform

Part-6:

The Challenge for Academic Research in Chemical Engineering



***“ Chemical Engineering
as an
Educational Discipline
has ceased to exist on the
100th Anniversary of AIChE ”***

Reuters News Service, November 2008

1. Knowledge as the Pivotal Element

- ❖ A Product-Centered Chemical Company is a Company that Generates New and Manages effectively existing Knowledge
 - Scientific, Technological, Marketing, Social, Political, and other type of knowledge
- ❖ Is Chemical Engineering Research in academic institutions generating
“Knowledge with Impact” ?

1. *Knowledge as the Pivotal Element* (Academic Impact and Industrial IP)

“First-to-Patent not First-to-Market” Coincidence of R&D and IP Strategies

- ❖ **Analysis of 500 industrial patents (1996-2002)**
 - 4 US Chemical Companies;
 - High index of scientific cutting edge patents (MIT index)
 - Chemicals, Materials, Product and Process patents
- ❖ **Citations of academic research:**
 - 19 % of citations were academic research papers
 - Only 0.3% of citations were from Chemical Engineering published research papers.

1. *Knowledge as the Pivotal Element* (Academic Impact and Industrial IP)

❖ Patent Productivity of Academic Research

- 5 chemical engineering departments
- 4 chemistry departments
- 3 departments of materials sciences
- Period: 1976-2002

❖ Productivity (no. of patents/faculty, year)

- Materials Science = 0.3 – 0.4
- Chemistry = 0.2 – 0.3
- Chemical Engineering = 0.08 – 1.2

(One dept = 0.25)

2. *The “Hidden Cost” of Research*

A List of Industrial, Truly Difficult, Technological Problems Exists



Who Is Working on Solving them ?

Is the academic world ready to “listen” (really) to the exciting industrial challenges and try to have an impact in addressing them?

3. *Inter-Disciplinary Research*

- ❖ Who is going to teach us how to do it?
 - “Inter-disciplinary” research is more than “collaborative” research
 - Crossing disciplinary segments, with tangible impact, is not yet visible

- ❖ Who is going to show us how to assign IP rights in inter-disciplinary research?
 - Serious handicap

4. *PSE in a Product-Centered Industry*

- ❖ Many “Products” are Processes in themselves. Why has Process Systems Engineering missed the chance to lead the engineering and manufacturing of such systems?
- ❖ Is PSE prepared to teach us how to engineer (design and manufacture) products, or should someone else do it?
 - The experience of discrete-parts’ product design and manufacturing (Mechanical Engineering)

5. *Future*

The Product-Oriented Character of the
Chemical Industry
is the best chance for
Academic Chemical Engineering
to become
Engineering
again

I suspect that the young of researchers of
AIChE 20 are instinctively following this path

Part-6:

Summary and an Exhortation

Summary

- ❖ Chemical companies are becoming progressively more “Product-and-Service Centered”.
- ❖ This shift requires a profound change in their “Corporate Culture” and “Operational Style”, and they are ill-prepared for it.
- ❖ Academic Chemical Engineering is also ill-equipped to address the new educational and research needs.
- ❖ The “War for Talent” will be very fierce and will determine winners and losers.

An Exhortation

(Paraphrasing Roger Sargent)

My address ...was frankly an exhortation, and today, perhaps in keeping with the general mood of our profession, it is a clear warning:

If we don't follow the dictates of our times and set about building the
Product-Centered future of Chemical Engineering,
as an
Engineering Discipline
again,
soon we are not going to have one!

"Is there a future for chemical engineering?", R. Sargent, 1977.

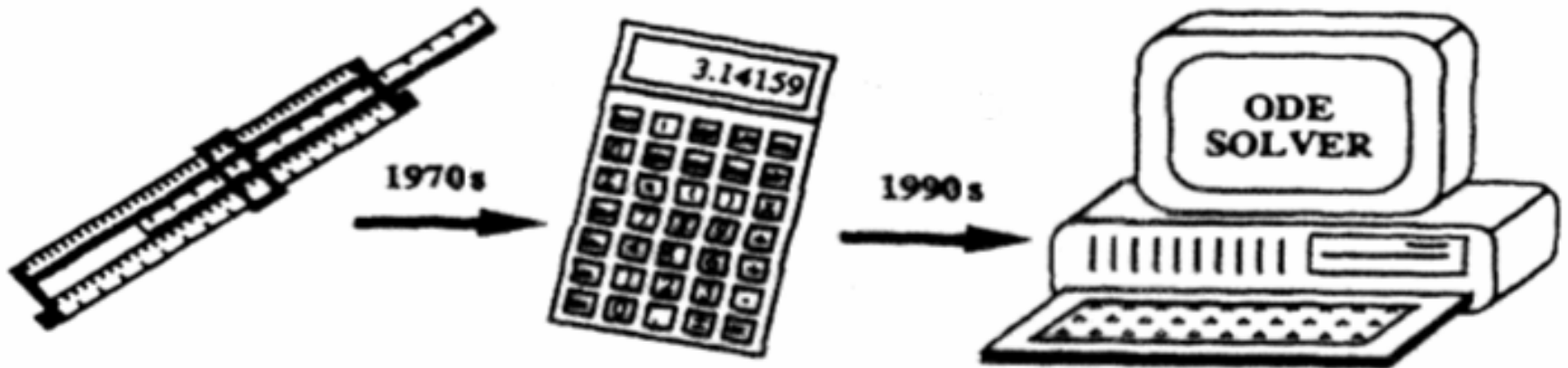
“Computing Through the Curriculum: An Integrated Approach for Engineering”

Thomas F. Edgar
Department of Chemical Engineering
University of Texas
Austin, TX 78712

ASEE Presentation - 6/23/04
Salt Lake City, UT

Outline

- The Engineering Computer Experience (and Problem-Solving)
- Industrial Practice
- Use of Software Tools
- Integration of Computing in the Curriculum
- Future Trends
- Conclusions



Paradigm shifts in engineering education.

To Compute (or Not)?

- Before 1970 computing in the curriculum was driven by faculty research that required computing.
- Undergraduate computing in the 1970s was often mostly concentrated in senior courses (e.g., design and control).
- In the 1980s computing was selectively introduced into sophomore and junior courses.
- In the 1990s some textbooks appeared with associated courseware.
- In the 21st century, the computer as a productivity tool is ubiquitous. Computing in the curriculum is not. Some faculty still believe any computing detracts from learning the concepts in their courses.

Desirable Attributes of Graduates

- Engineers are fundamentally problem solvers, seeking to achieve some objective of design or performance among technical, social, economic, regulatory, and environmental constraints.
- Graduates should have a grasp of fundamentals and engineering tools, enabling them to specialize or diversify as opportunity and initiative allow.

- Professional attributes should be cultivated, such as willingness to make estimates and assumptions, readiness to face open-ended problems and noisy data, and a habit of visualizing the solution.
- Professional skills include problem solving; estimating uncertainty; using computational tools; economic analysis; and the ability to plan, execute, and interpret experiments.
- Graduates should be able to integrate knowledge and information to aid in solution of chemical engineering problems.

Goals in Teaching Computing To Undergraduates

- Learn fundamental knowledge of computing, programming and computers
- Gain awareness of and preparation in emerging aspects of computing
- Mesh with computing requirements in the other courses of the curriculum
- Match knowledge and skills required by engineers in their day-to-day professional lives
- Open the door for further study and specialization in computing-related areas
(source: University of Colorado)

The Engineering Computing Experience

- When should computing be introduced to the engineering student?
- How much formal programming instruction on languages such as C should be provided (vs. usage of computing tools such as MATLAB, spreadsheets, etc.)?
- Is a numerical methods course required and when does this occur in the course sequence? How many credit hours are needed?
- Should every course include some computing?

Teaching Computer Programming

- Taught in engineering departments (1960-1980).
- Most engineering degree plans in 1980s changed to “CS 101” course.
- Catalyzed by growth in Computer Science programs across the U.S.
- Has migrated through several incarnations (Fortran, Pascal, C, C++, Java, etc.)
- Should it be taught by computer science or engineering faculty?

“CS 101” Advocates

- Engineers should learn fundamental concepts of programming and computer science.
- Computing should be taught by computer scientists, not engineers.
- Engineering faculty are not interested in teaching computing languages to their students.
- These courses involve a significant number of semester credit hours (SCH) and budgetary resources.

Engineering Tools Approach

- Engineering students need a solid grounding in problem-solving with modern computing tools.
- Engineering students need the knowledge and tools required in their professions.
- Engineering computing and problem-solving are best taught by engineers in the context of an application.
- No room for separate 3 or 4 SCH course in programming.

The New Digital Generation (B.S. Engineering, 2010)

- Lives with pervasive microprocessors and telecommunications (e.g., cell phones)
- Napster, Playstation, Pokemon
- Demands computer interaction, plug and play
- Learns through experimentation, group interaction, intuition
- Focuses on future practical goals

The New Student Knows How to Use Computers and the Internet

A survey of 804 10-17 year olds in Silicon Valley in Fall 2002

- 83-86% go to public school.
- 99% have used a computer; 83% of those by the age of 10.
- 93% have been online; 86% of those by the age of 11.
- 63% have an internet-connected computer in their bedroom.
- 5.5 hours is the mean average hours spent online weekly.
- 72% use instant messaging one or more times/week.
- 96% think knowing how to use computers and the Internet is very or somewhat important to their future education.

San Jose Mercury News, 5/03.

Computing Roadblocks

- High school preparation level varies widely.
- Programming is a skill that must be used every semester.
- Use of computers in science and math courses is extremely uneven and unpredictable.
- A freshman engineering computing experience is one solution if department has the instructional capability.

Introductory Computing Course – An Outline

- Problem-Solving: engineering method, units, precision in calculations
- Symbolic Computing: algebra, calculus
- Spreadsheet Techniques: solutions to engineering problems, VBA in Excel
- Programming Fundamentals: data types, program-flow, modularity, object-oriented features
- Elementary Numerical Methods: linear, nonlinear equation solving, linear regression
- Software Tools: MathCAD, MATLAB, Excel

What Students Learn From Writing Computer Programs

- What assumptions go into the program
- What the right answer should be
- What is the input, what is the output
- Clear organization of thought, logic, and calculations
- Errors can exist in a program
- Programming is unforgiving for ambiguities and errors

Why Did You Switch From C++ to MATLAB?

- Interpreted language (write, debug, run in same environment)
- Editor can pass code directly to MATLAB application
- Graphical interface (2-D, 3-D)
- Numerical analysis
- Ease of use, widespread availability, student package is powerful enough for education

Programming Features of MATLAB

1. Loops (for, while)
2. Conditional statements (if)
3. Relational operations (\leq , etc.)
4. Logical operations (AND, NOT)
5. Matching
6. I/O
7. Modularity
8. Error processing
9. Array math

Faculty Foibles

- Faculty often confuse what is important for their students vs. for themselves.
- Faculty computing needs often align with their research interests (vs. undergraduates).
- They may be out of touch/out of date on computing practices.
- Their own computer skills may be “oxidized.”
- Computing (and programming) is not part of their daily professional existence (and is not expected to be).
- Perceived computing needs are not connected to current knowledge of industrial computing practice.

How Recent ChE Graduates Use Computing

A CACHE Survey
2003

Target Audience: Received B.S.
in Engineering Between 1998
and 2003

Total Number of Responses

293

Participating Universities: Carnegie Mellon
University, Clarkson University, McMaster University,
University of Texas at Austin

Computing in Industry

Type of work (highest priority)

	<u>2003</u>
• R & D	25.1% (69)
• Plant/Process Support	21.8% (60)
• Process Design/Analysis	17.5% (48)
• Process Control	7.6% (21)
• Administrative	4.7% (13)
• Systems	2.2% (6)
• Other	21.1% (58)

Fraction of Day at the Computer

	<u>2003</u>	<u>1997</u>
• 0 to $\frac{1}{4}$	9.7% (28)	19%
• $\frac{1}{4}$ to $\frac{1}{2}$	21.9% (63)	36%
• $\frac{1}{2}$ to $\frac{3}{4}$	25.7% (74)	26%
• $\frac{3}{4}$ to 1	28.5% (82)	17%
• All day	14.2% (41)	2%

Computer use for office tasks (e-mail, word processing, the web, etc.)

	<u>2003</u>	<u>1997</u>
• Yes	99.7% (288)	95%
• No	0.3% (1)	5%

Use of Spreadsheet Programs (e.g., Lotus 1-2-3, Excel, Quattro Pro, etc.)

2003

- Yes 98.3% (282)
- No 1.7% (5)

Most popular spreadsheet program: **Microsoft Excel**

Purposes of Spreadsheet Programs (Overlapping)

- Data Analysis 88.2% (253)
- Numerical Analysis 47.4% (136)
- Material Balances 25.1% (72)
- Economic Studies 23.7% (68)
- Other (e.g., reporting, financial modeling, emissions calculations, etc.) 16.7% (48)

Other Software Packages

Dedicated Statistical Software

- Yes 26.9% (77)
- No 73.1% (209)

Most popular among users: **JMP**

Others: SAS, MiniTab

Numerical Analysis Software

- Yes 25.5% (73)
- No 74.1% (212)

Most popular among users: **MATLAB**

Others: MathCad, Octave

Database Management Systems

- Yes 65.6% (187)
- No 34.4% (98)

Most popular among users: **Access**

Others: Oracle, SQL

Symbolic and Mathematical Manipulation Software

- Yes 10.1% (29)
- No 89.9% (257)

Most popular among users: **Mathematica**

Others: Maple, MathCAD

Numerical Methods Libraries

- Yes 6.3% (18)
- No 93.7% (266)

Most popular among users: **IMSL**

Others: DASSL, LAPACK

Training

Initial time needed to learn computer skills for job function

	<u>2003</u>	<u>1997</u>
• < 1 month	60% (171)	72%
• 1 – 3 months	18.9% (54)	17%
• 3 – 6 months	9.8% (28)	4%
• > 6 months	4.9% (14)	2%
• Don't Know	6.0% (17)	5%

Primary Source of Training

	<u>2003</u>	<u>1997</u>
• Self	71.3%	58%
• Colleagues	14.3%	16%
• Organization	8.6%	16%
• Others (Training Companies, Tool Vendor, School, etc.)	5.7%	10%

Adequate training at university to use and understand process simulation programs:

• Yes	49.1%
• No	21.6%
• No opinion	29.3%

Computer Programming

Asked to write computer programs at work:

	<u>2003</u>	<u>1997</u>
• Yes	38.2% (109)	20%
• No	61.8% (176)	80%

Most common programming language: **Visual basic**

Should at least one programming language be required at undergraduate level?

• Yes, it's important	78.2% (223)
• No, it's not necessary	13.3% (38)
• No opinion	8.4% (24)

Programming Language Recommended

- Visual Basic 32.6% (73)
- Does not matter 28.1% (63)
- C++ 21.4% (48)
- Java 5.4% (12)
- Fortran 77 2.2% (5)
- C 2.2% (5)
- Fortran 90 2.7% (6)
- Pascal 1.3% (3)
- Other 4.0% (9)

Programming Languages

Expected by employer to be competent in a programming language:

	<u>2003</u>	<u>1997</u>
• Yes	27% (76)	12%
• No	73% (206)	88%

Expected to be literate in different computer languages:

	<u>2003</u>	<u>1997</u>
• Yes	14.1% (40)	8%
• No	85.9% (243)	92%

Numerical Software Tools Used in Engineering Departments

- MATLAB
- MathCAD
- Mathematica
- Maple
- TK Solver
- Excel

At many schools, Excel is not formally taught but expected to be used.

Industrial Usage of Excel

- Dominant software package used in industry
- Fits the nature of many calculations performed by engineers in industry
- Can be readily used with Visual Basic (difficult to analyze spreadsheet logic)
- May encourage the use of inaccurate or inefficient numerical calculations
- Does not necessarily suggest that sound numerical approaches should be de-emphasized at universities

Observations by a Faculty Curmudgeon

Today's students

- Are an impatient culture
- Prefer sound-bite answers
- Do not want to engage in a methodical analysis
- Do not enjoy deriving equations
- Say “don't tell me why, tell me how”

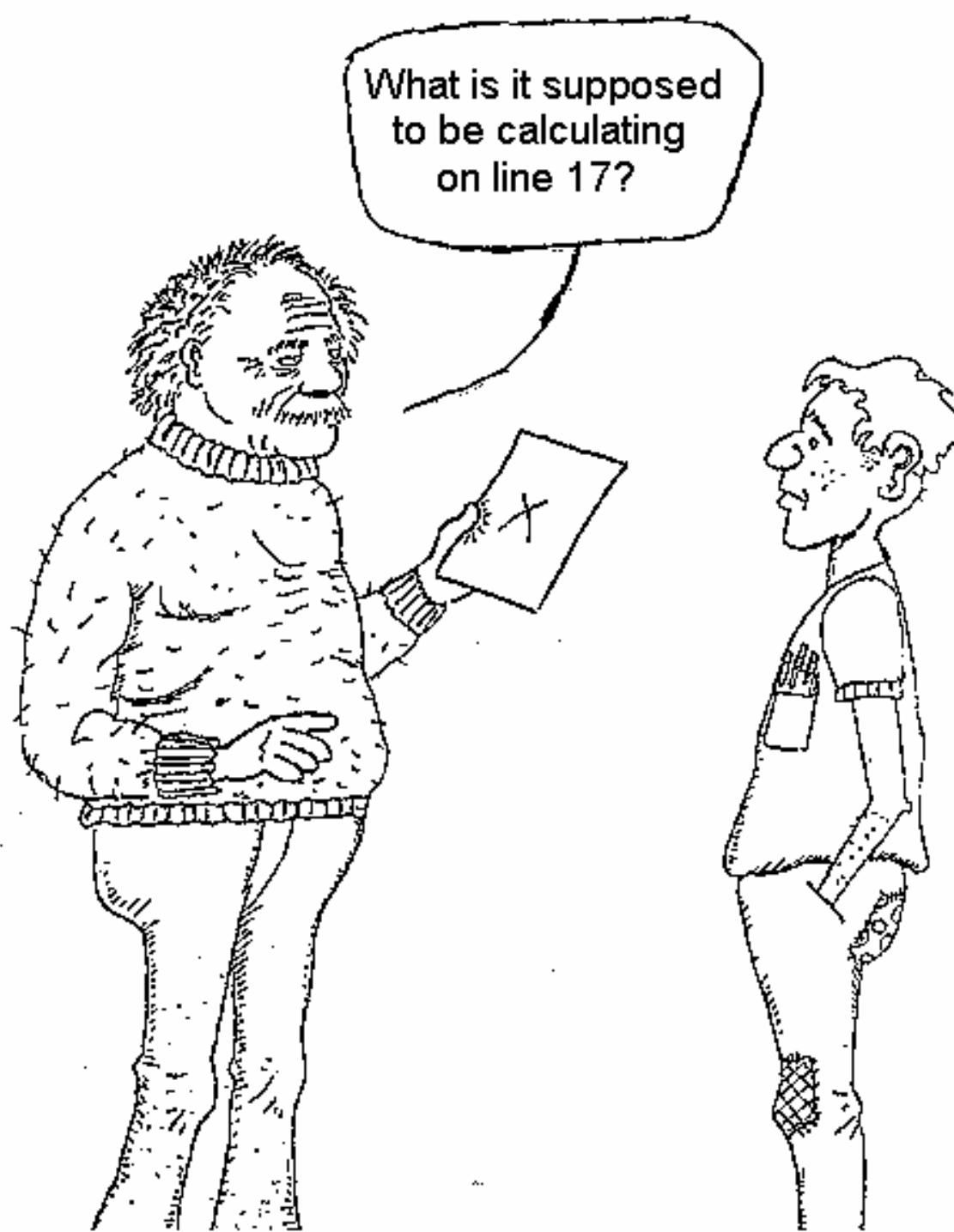
IT Laws

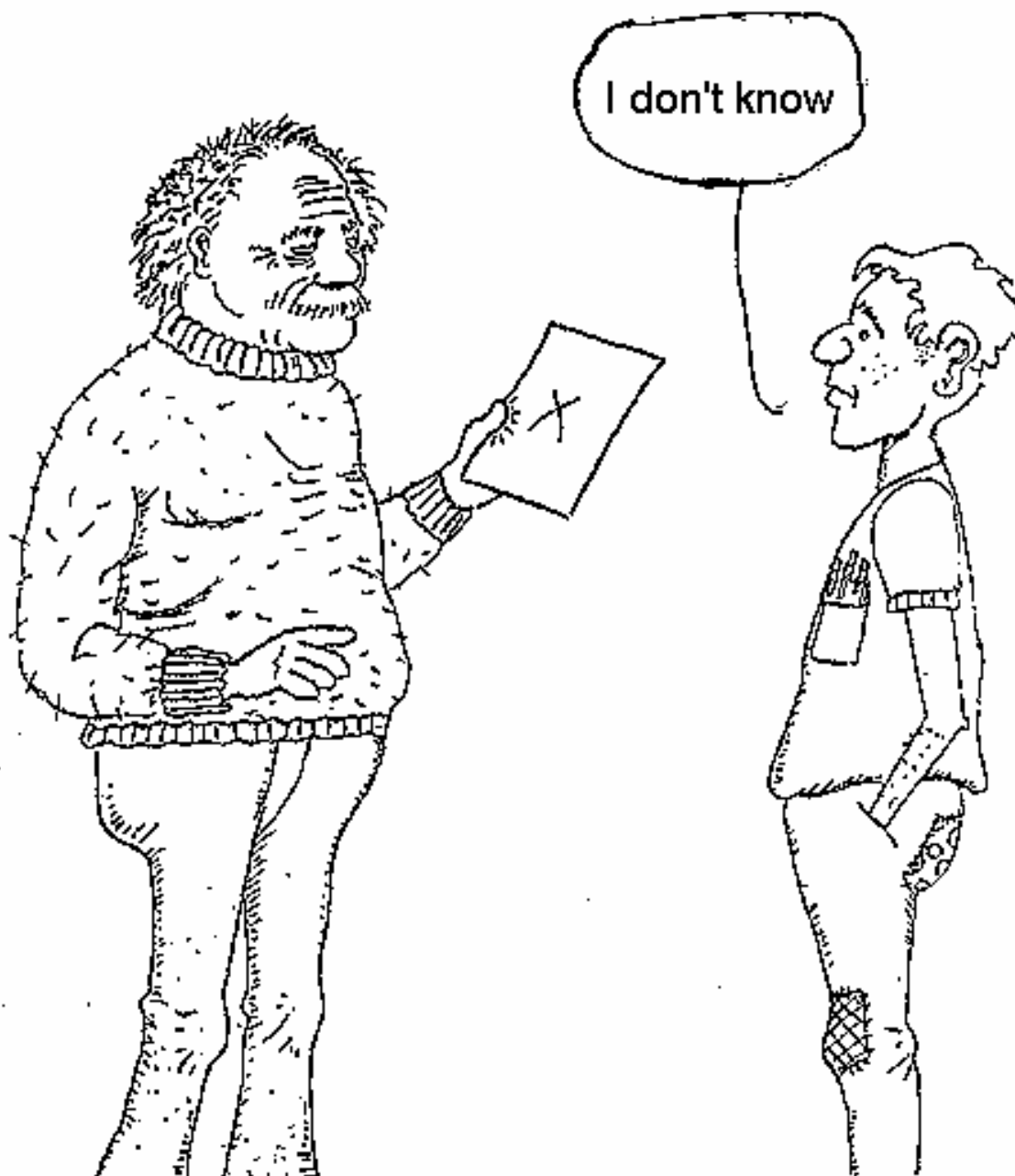
- If it's not on the web, it's not true.
- If it is on the web, it might not be true.
- If the answer is produced from software, it must be correct (any may contain a large number of significant digits).

The Danger of Productivity Tools (Software)

- Students may treat software as a black box (button-pushing or mouse-clicking without learning what is behind the button).
- Students have no idea of how to extend or modify the program.
- Students do not know how to estimate the order of magnitude of the answer (not from the slide rule era).
- Students have little sense of units and reasonable values for them.
- Numerical issues are pushed beneath the surface: e.g., accuracy, convergence, default parameters.







NASA: Human error caused loss of Mars orbiter

November 10, 1999

Web posted at: 4:27 p.m. EST (2127 GMT)

In this story:

[Report Summary](#)

[Signs of trouble came early](#)

[Will Polar Lander be safe?](#)

[RELATED STORIES, SITES](#) ↓

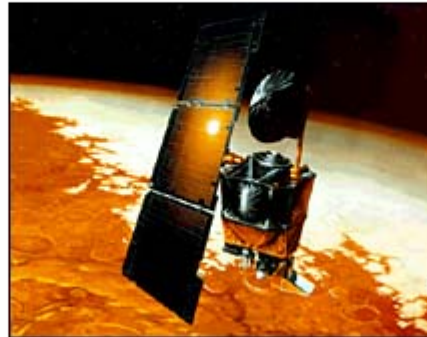


Illustration of the Mars Climate Orbiter

WASHINGTON (CNN) -- Failure to convert English measures to metric values was the root cause of the loss of the Mars Climate Orbiter, a spacecraft that smashed into the planet instead of reaching a safe orbit, a NASA investigation concluded Wednesday.

In a scathing report released Wednesday, an investigation board concluded that NASA engineers failed to convert English measures of rocket thrusts to newton, a metric system measuring rocket force.

One English pound of force equals 4.45 newtons. A small difference between the two values caused the spacecraft to approach Mars at too low an altitude and the craft is thought to have smashed into the planet's atmosphere and was destroyed.

Integration of Computing Through the Curriculum

- Introduction to Professional Area (Freshman)
- Introduction to Computing (Freshman)
- Numerical Methods (Sophomore)
- Statistics (Junior)
- Laboratory Experiences (Junior/Senior)
- Simulation (Junior/Senior)
- Design (Senior)
- Control (Senior)
- Electives (Senior)

How many different software packages are required?
Are textbooks tied to software?

Too Many Tools? A Chemical Engineering List

Word/Powerpoint

Excel

MathCAD

MATLAB

Mathematica

Simulink

Polymath

EZ-Solve

HYSYS

Aspen Plus

Minitab

JMP

Control Station

LabView

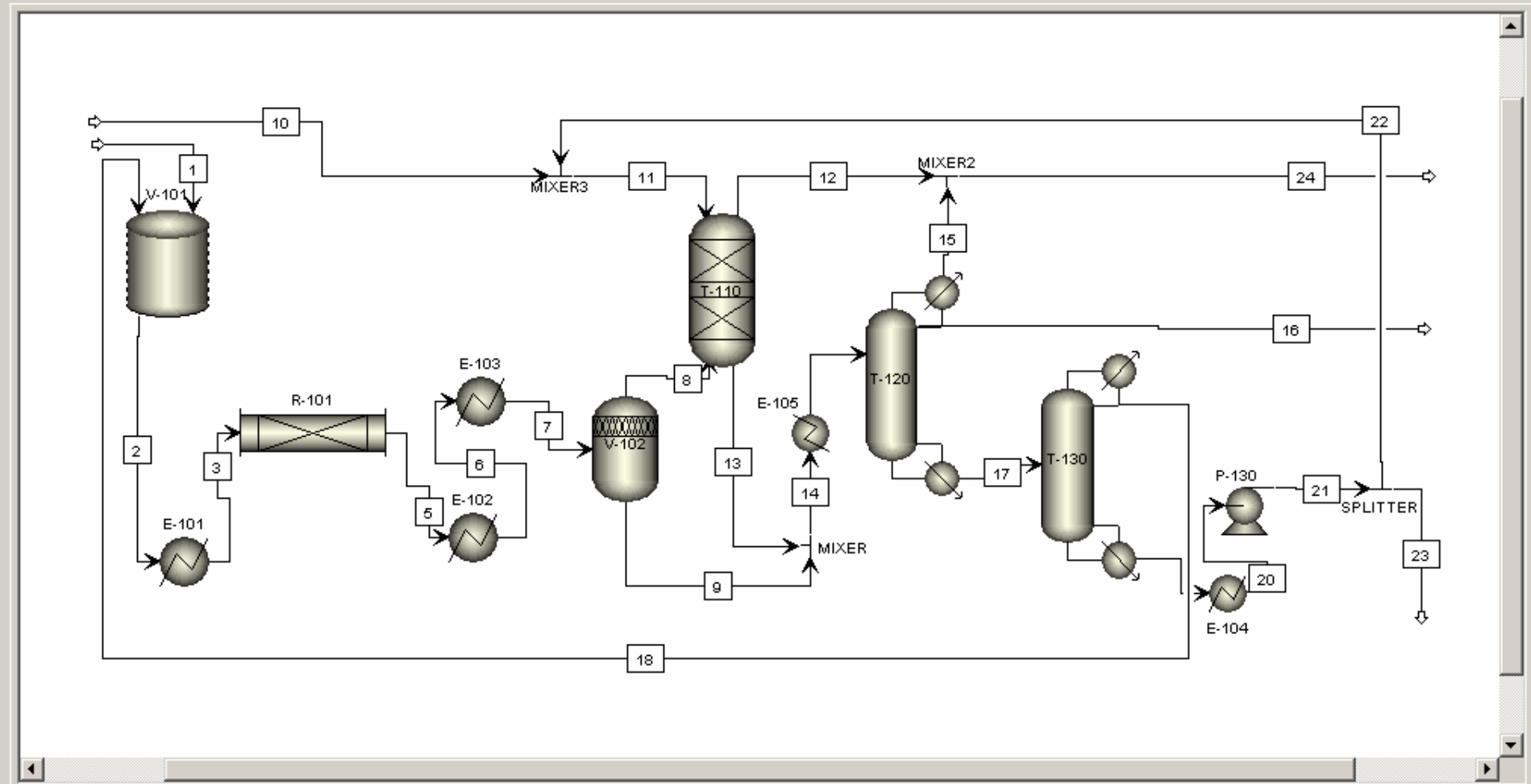
LadSim

AutoCAD

Examples of Commercial Simulation Packages in Education

- ECE: PSpice, LabVIEW
- ME: ANSYS
- ASE: NASTRAN
- CE: Structural MathCAD
- ChE: HYSYS, Aspen Plus

Several ChE departments (e.g., VPI, Rowan) have used the Aspen Plus simulator throughout sophomore, junior and senior courses.

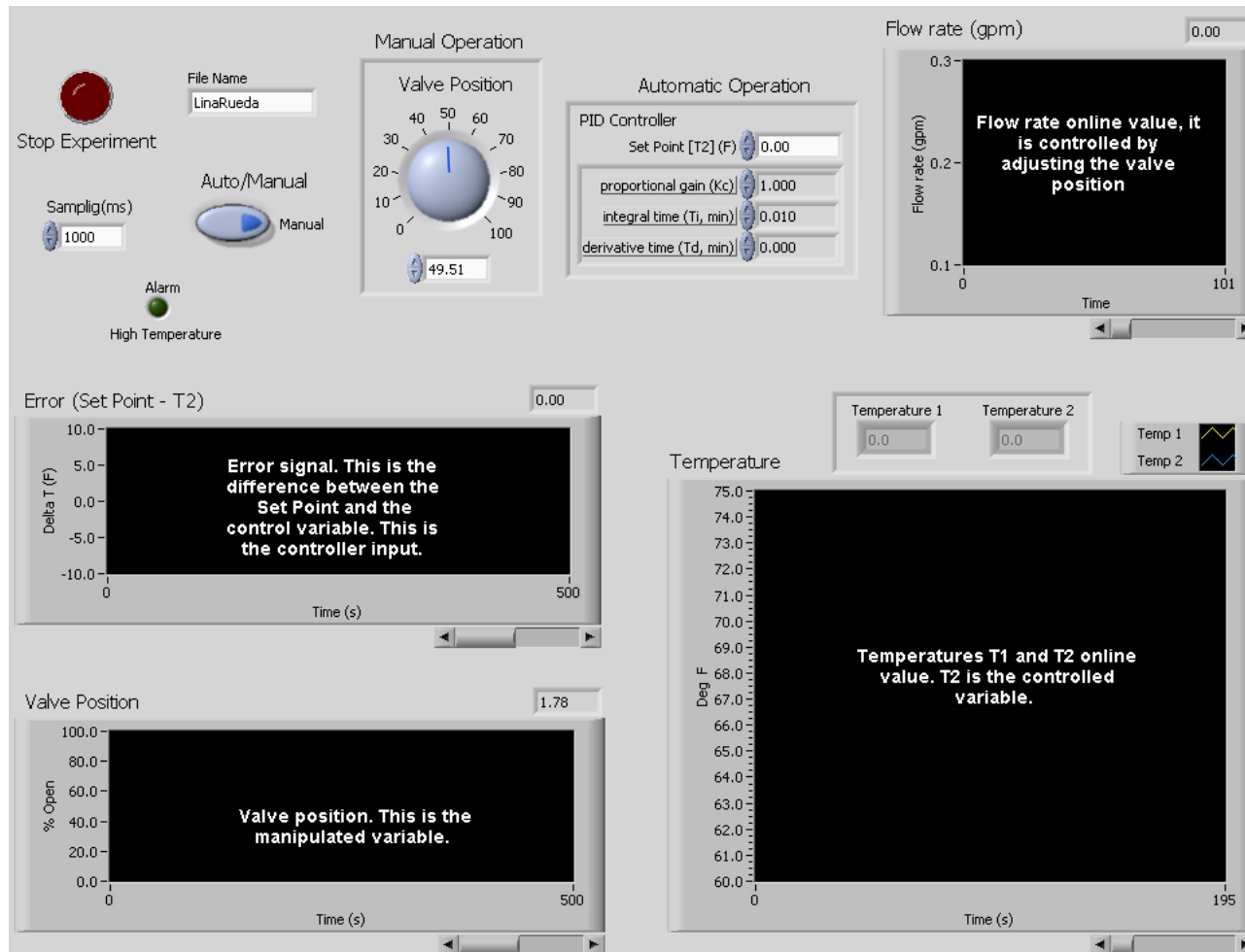


Process Flo...

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models



Computer Interface -2



Faculty Control vs. Department Control

- One view: professor is a “high priest” and has discretion to select course content and textbook (in the name of academic freedom).
- The Department Chair/Department Curriculum Committee may or may not be able to influence course content.
- Tight coupling of prerequisite courses in engineering makes independent operation infeasible, especially in outcome-based ABET 2000 (KAS).
- Compromise: 80% of content determined by Department consensus on prerequisite material (20% left to instructor).
- Content includes role of computing.

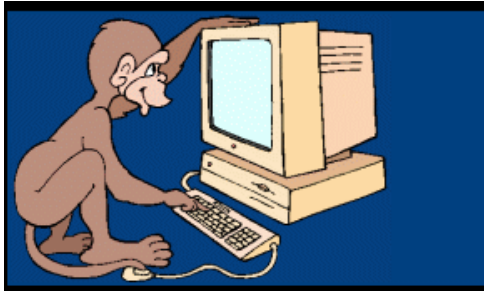
“Changing the curriculum is like moving a graveyard-you never know how many friends the dead have until you try to move them.”

Calvin Coolidge or
Woodrow Wilson

“Let sleeping dogs lie.”



The Non-integrated Curriculum Approach?



The Monkey Shakespeare Simulator

"If you have enough monkeys
banging randomly on typewriters,
they will eventually type the works
of William Shakespeare."



Techniques to Build Faculty Consensus on Computing

- Need a champion (or two), not necessarily Department Chair (although you want his/her support)
- Perform a software audit of all courses to identify any common threads.
- Hold half-day retreats each semester or year; form working groups based on curricular areas.
- Set up faculty lunches or meetings once per month to walk through the curriculum.

FLOWCHART

CATALOG: 2000-2002, 2002-2004

ALWAYS REFER TO THE CURRENT
COURSE SCHEDULE FOR THE MOST
UP-TO-DATE PREREQUISITES

LEGEND

DEPT. & COURSE NO.	COURSE TITLE
PRE	CO
ALL PREREQS. LISTED HERE GRAY - C OR BETTER REQ. WHITE - PASS REQ.	ALL COREQS. LISTED HERE

Student Name: Computing in ME
UT EID: _____

1 16 HRS.	M 408C DIFFERENTIAL & INTEGRAL CALCULUS NOTE M 408C + M 408D M 408C + M 408D + M 408E	CH 301 PRINCIPLES OF CHEMISTRY I	ME 302 INTRO TO ENGRG DESIGN & GRAPHICS CAD Pro Engrg Intro to FEA CO *	RHE 306 RHETORIC & COMPOSITION	SOC. SCI. APPROVED SOCIAL SCIENCE ELECTIVE NOTE SEE APPROVED LIST IN ME HANDBOOK OR OUTSIDE ETC 3.23H
2 16 HRS.	M 408D SEQ. SERIES & MULTIVAR. CALCULUS PRE * M 408C	PHY 303K ENGINEERING PHYSICS I PRE * CO M 408C/K PHY 103M M 408L	PHY 103M LABORATORY FOR PHY 303K CO PHY 303K	ME 205 COMPUTERS & PROGRAMMING C++ ML Online self-paced CO * M 408C/K	GOV 310L TEX & AMERICAN GOVERNMENT NOTE 12 HOURS REQD.
3 17 HRS.	M 427K ADVANCED CALCULUS FOR APPLICATIONS I PRE * M 408D/L	PHY 303L ENGINEERING PHYSICS II PRE * CO * M 408D/L PHY 303K PHY 103M M 408M	PHY 103N LABORATORY FOR PHY 303L CO PHY 303L	ME 326 THERMODYNAMICS PRE * M 408D CH 301 PHY 303K	EM 319 MECHANICS OF SOLIDS PRE * M 408D/L EN 306
4 16 HRS.	ME 311 MATERIALS ENGINEERING PRE CO CH 301 ME 306 ME 326 EN 319	ME 111L MATERIALS ENGINEERING LAB CO ME 311	ME 218 ENGINEERING COMPUTATION METH. PRE ME 205 M 407E	ME 330 FLUID MECHANICS PRE CO M 407E EN 301 ME 304	ME 130L FLUID MECHANICS LAB CO M 408D EN 306
5 17 HRS.	ME 336 MATERIALS PROCESSING PRE CO EN 319 ME 311 ME 111L	ME 136L MATERIALS PROCESSING LAB PRE CO ME 111L EN 319	ME 338 MACHINE ELEMENTS PRE ME 311 EN 319	ME 339 HEAT TRANSFER PRE CO ME 218 ME 330 ME 130L ME 139L	ME 139L HEAT TRANSFER LAB CO ME 339
6 14 HRS.	ME 353 ENGINEERING ECONOMIC ANALYSIS PRE * ME 205 M 408C ME 336	ME 333T ENGINEERING COMMUNICATIONS PRE RHE 306	ME 344 DYNAMIC SYSTEMS & CONTROLS PRE M 427E ME 218 ME 324	ME 343 THERMAL FLUID SYSTEMS PRE ME 339 ME 139L	2 HR. ATAE APPROVED TECH AREA ELECTIVE NOTE ACM, TO MATH REQ. REQ. SELECT AREA, ADVISOR, & MEET TO APPLY COURSES
7 16 HRS.	ME 360J DESIGN METHODOLOGY PRE ME 302 ME 330 ME 336 ME 139L ME 333T ME 338 ME 339 ME 353	ME 244L DYNAMICS SYSTEMS & CONTROLS LAB PRE CO ME 238 ME 344	3 HR. ATAE APPROVED TECH AREA ELECTIVE NOTE ACM, TO MATH REQ. REQ. SELECT AREA, ADVISOR, & MEET TO APPLY COURSES	2 HR. ATAE APPROVED TECH AREA ELECTIVE NOTE ACM, TO MATH REQ. REQ. SELECT AREA, ADVISOR, & MEET TO APPLY COURSES	3 HR. MATH MATH ELECTIVE NOTE SEE APPROVED LIST IN ME HANDBOOK OR OUTSIDE ETC 3.23H
8 16 HRS.	ME 266K MECHANICAL ENG. DESIGN PROJECT PRE ME 343 ME 344 ME 244L ME 360J	ME 266P MECHANICAL ENG. DESIGN PROJECT CO ME 266K	3 HR. ATAE APPROVED TECH AREA ELECTIVE NOTE ACM, TO MATH REQ. REQ. SELECT AREA, ADVISOR, & MEET TO APPLY COURSES	3 HR. M/NS MATH/ NATL. SCI. ELECTIVE NOTE SEE APPROVED LIST IN ME HANDBOOK OR OUTSIDE ETC 3.23H	GOV 312L AMERICAN GOVERNMENT PRE NOTE GOV 310L

BASIC SEQUENCE

MAJOR SEQUENCE

ML, Labview

Electives: ANSYS, Fluent, other simulation packages

- A core group of faculty who teach computing-oriented courses should agree on key tenets.
- They can invite faculty who teach courses that do not use much computing for a discussion on integration.
- Challenge faculty who do not use computing tools to be creative in adding such content.
- This dialog may pinpoint curriculum modifications or changes in prerequisites for certain courses.

Disciplinary Cooperation Can Address Computing in the Curriculum

Founded in 1969, CACHE is a not-for-profit organization whose objectives are to make chemical engineering instruction more effective and to enhance the productivity of students, educators, and practitioners with computer-based tools and technology.

CACHE works with:

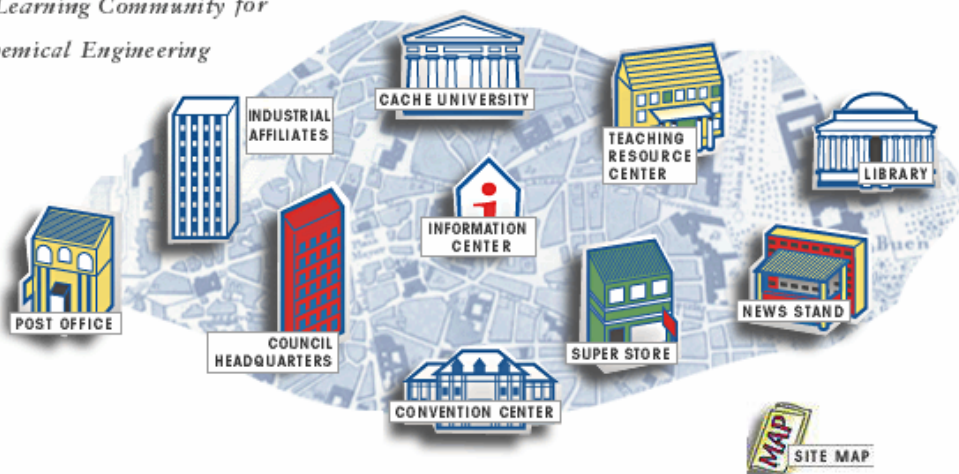
- 140 ChE Departments
- 28 Trustees
- 12 Industrial Affiliates
- Professional Societies such as AIChE and ASEE
- www.cache.org



A Learning Community for
Chemical Engineering

Search

[Advanced Search](#)



Map key

INFORMATION CENTER	CACHE NEWS STAND	TEACHING RESOURCE CENTER	CACHE UNIVERSITY	DIGITAL LIBRARY RESOURCES	SUPER STORE CACHE PRODUCTS	CONVENTION CENTER	INDUSTRIAL AFFILIATES	COUNCIL HEADQUARTERS	POST OFFICE
CACHE	CACHE News: Spring 2002 and previous issues.	Curriculum resources on the Web.	Online course content for ChE's	General Web resources for ChE's, useful links.	Software and publications, including POLYMATH	Research Conferences: FOCAPD, FOCAPD, FOMMS, CPC, and others	Industrial Affiliates and supporting academic departments	Board of Trustees info	Contact info for CACHE

Optimized for 4.0 browsers. Click on "site map" to view a text-based list of categories.

Click [here](#) to go to the Fall 2003 Newsletter.

WORKSHOP - JUNE 20, 2004 - [Spreadsheet Problem Solving for ChE Faculty](#)

[Chemical Engineering Faculty Openings / "Meet the Faculty Candidates" \(Resume Postings\)](#)

[CACHE Computing Survey Results](#)

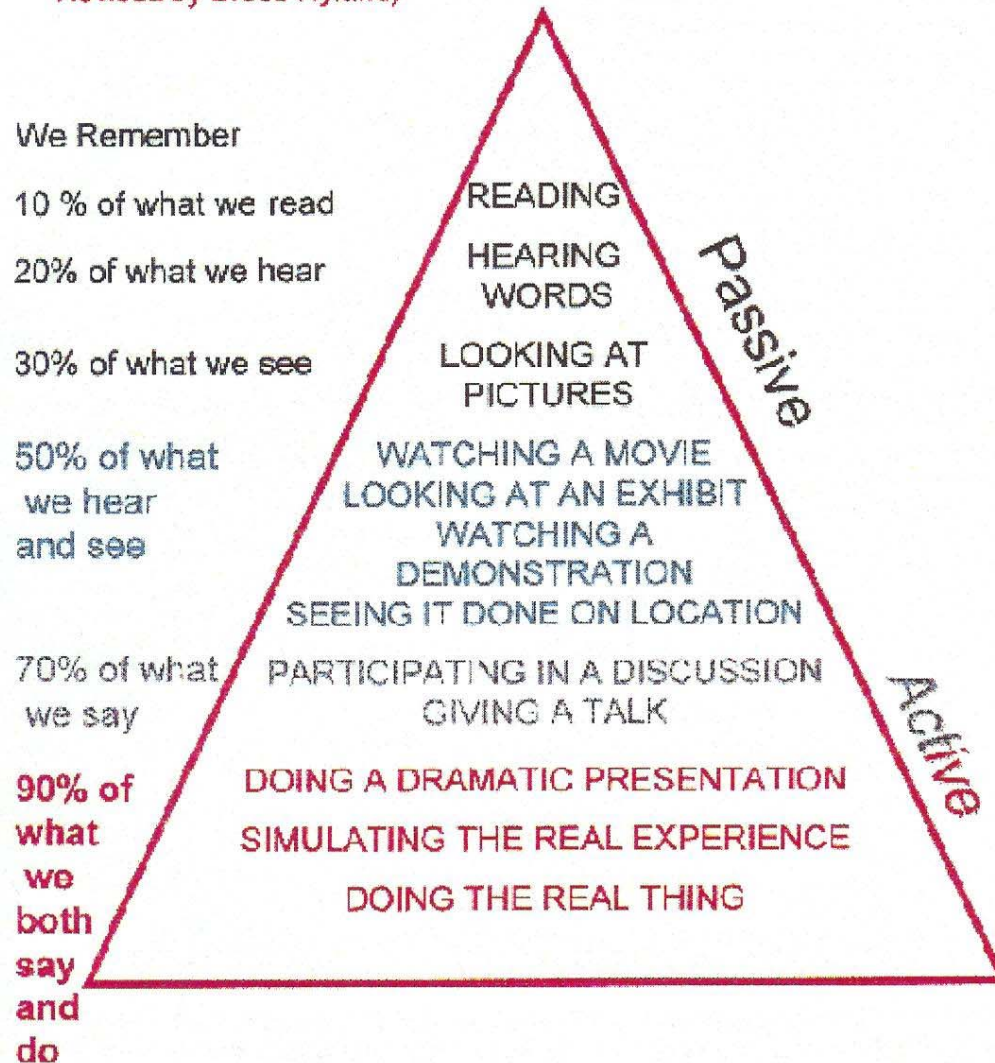
[ASEE Summer School Materials Available to Faculty](#)

Future Topics in Undergraduate Computing

- CFD(Computational Fluid Dynamics)
- Molecular Modeling and Product Design
- Curriculum Redesign

Active Learning

(based on Edgar Dales Cone of Experience
Revised by Bruce Hyland)



Some Quotes about Modeling and Computing

- All models are wrong but some are useful.
- It is much easier to prove a model wrong than prove it right.
- It is better for a model to be approximately right than exactly wrong.
- A model should be as simple as possible but no simpler.

- The purpose of computing is insight, not numbers.
- The purpose of computing numbers is not yet in sight.

(R. Hamming)

Numerical vs. Analytical Approaches in Modeling Physical Behavior

- Need to learn both approaches (advantages and disadvantages)
- Need to re-examine role of detailed analytical solutions (training for industry vs. graduate school)
- Use fewer simplifying assumptions in numerical solutions
- Public can run simulators in science museums, so engineering education can find a way
- Observations can come from physical experiments and numerical experiments

DISTRIBUTION OF HYDRAULIC CONDUCTIVITY AT THE FRENCH LIMITED SITE

Purpose

The purpose of this lab is to explore the soil conditions of the French Limited site and determine the distribution of the hydraulic conductivity of the uppermost soil layer.

Introduction

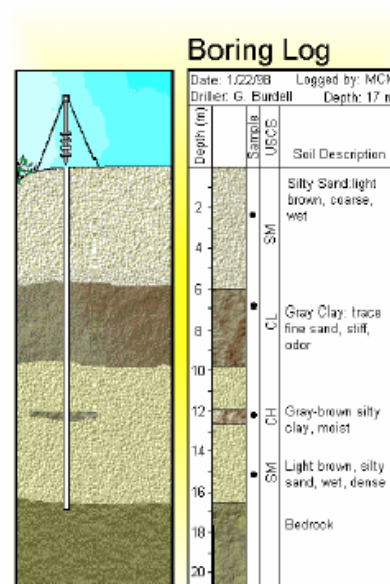
In order to explore the soil conditions at a site, civil engineers will often drill boreholes. Boreholes allow the engineer to determine the type and thickness of the soils (Figure 1). Soil samples may be taken during drilling so that tests may be performed on them in the laboratory.

One test that might be performed on a soil sample is a hydraulic conductivity test. Hydraulic conductivity (or K) characterizes how well a soil will transmit water. For example, the hydraulic conductivity is higher for sand than for clay, and water flows more quickly through sand than through clay. The units of hydraulic conductivity are the same as those for velocity, length divided by time. The value of hydraulic conductivity must be positive.

At the French Limited site, you are interested in the types of soils present and their hydraulic conductivities because you will want to determine if chemicals from the lagoon could travel through the subsurface and contaminate drinking water wells of the residents in the area. From previous research in the area of the French Limited site, you know that the groundwater generally flows toward the southwest. You also know that the following soil layers are generally present, from the surface down:

- Uncompacted sand with clay and silt.
- Sand with some gravel.
- Silty clay, silty-sandy clay, and clay.

An engineer from your firm previously explored the soil conditions at the French Limited site with 10 boreholes, taking soil samples and running hydraulic conductivity tests. You would like more information about the soil conditions and hydraulic conductivity, so you will explore the site with more boreholes.



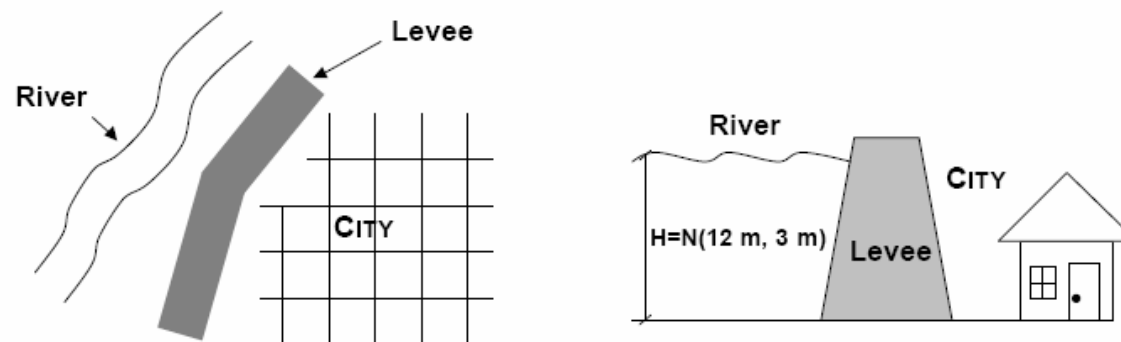
LEVEE DESIGN BASED ON THE BINOMIAL DISTRIBUTION

Purpose

You will be investigating how the height of a levee affects: (i) the performance over different design lives; (ii) the return period of the levee being overtopped; and (iii) the construction cost.

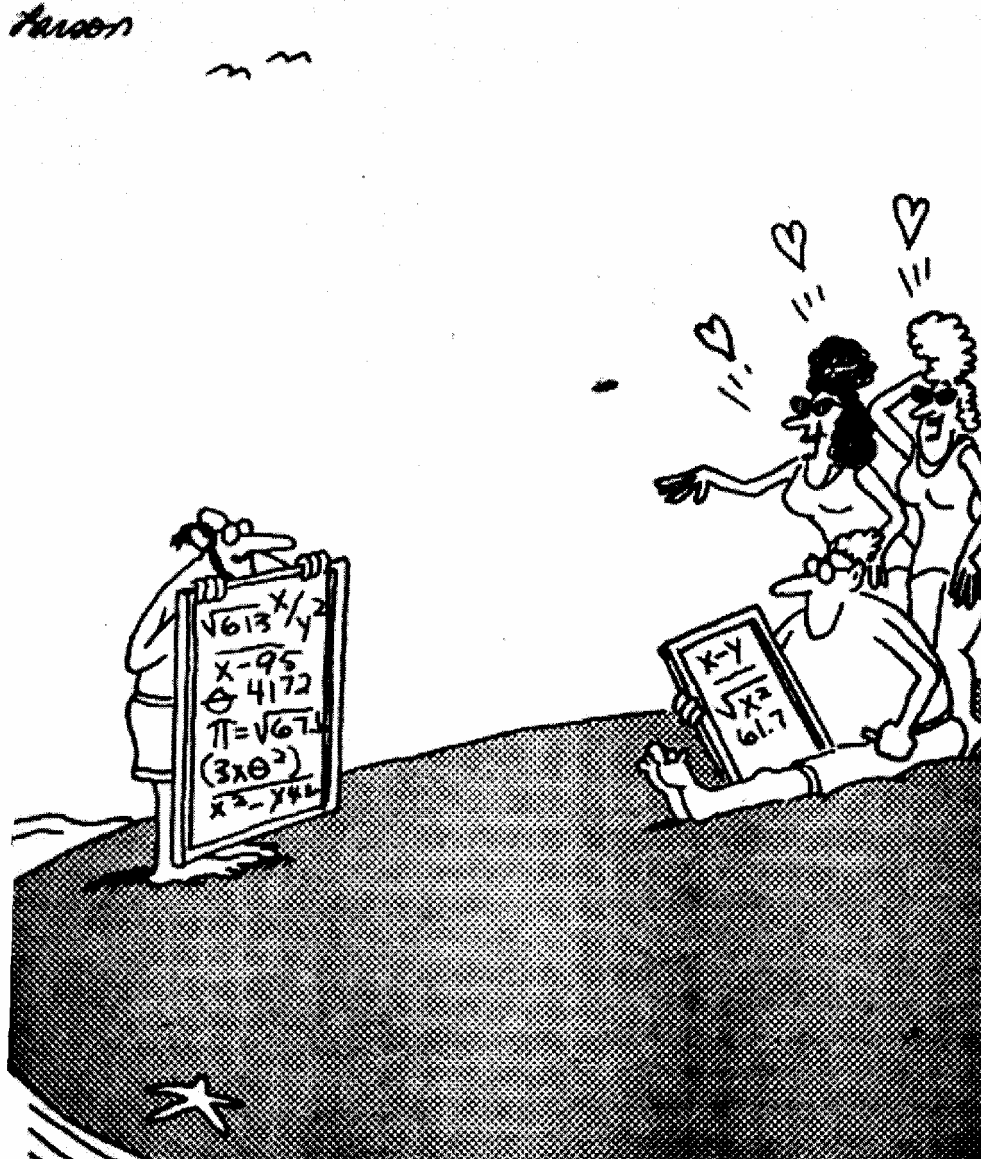
Introduction

Levees are constructed of compacted earthen materials and are built as flood control structures. The design height for the levee is usually based on the maximum annual flood level for the area. Also, the design height depends on the amount of money available to pay for construction and the amount of risk the client wishes to accept in the event that the levee fails.



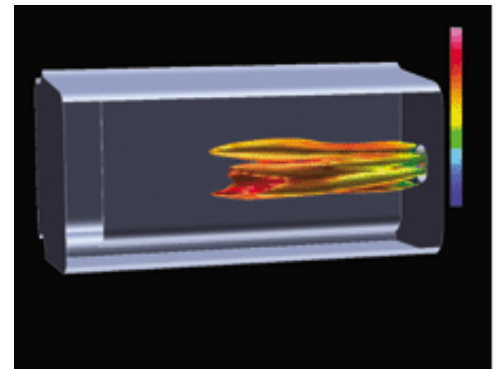
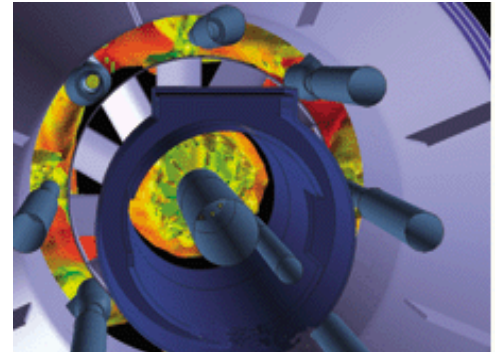
Both the federal government and state governments offer relief aid for areas destroyed by floods. However, the agencies controlling these funds have set specific standards to reduce the probability that an area will be flooded and, therefore, reduce the amount of money that they must give out. In order to be eligible for future Federal Emergency Monetary Assistance (FEMA) funds or equivalent state funds, the City of Anytown may need to upgrade their levee system. The current levee height is 15 meters and may not provide adequate protection against flooding. Based on historical records of the river heights, the maximum annual water height (H) has a normal distribution with a mean of 12 meters and a standard deviation of 3 meters. You have been hired by the city to evaluate if the current levee meets the qualifications for federal and/or state relief. You will also test different levee designs and evaluate the performance and costs of these designs for comparison.

The Lure of Advanced Computing

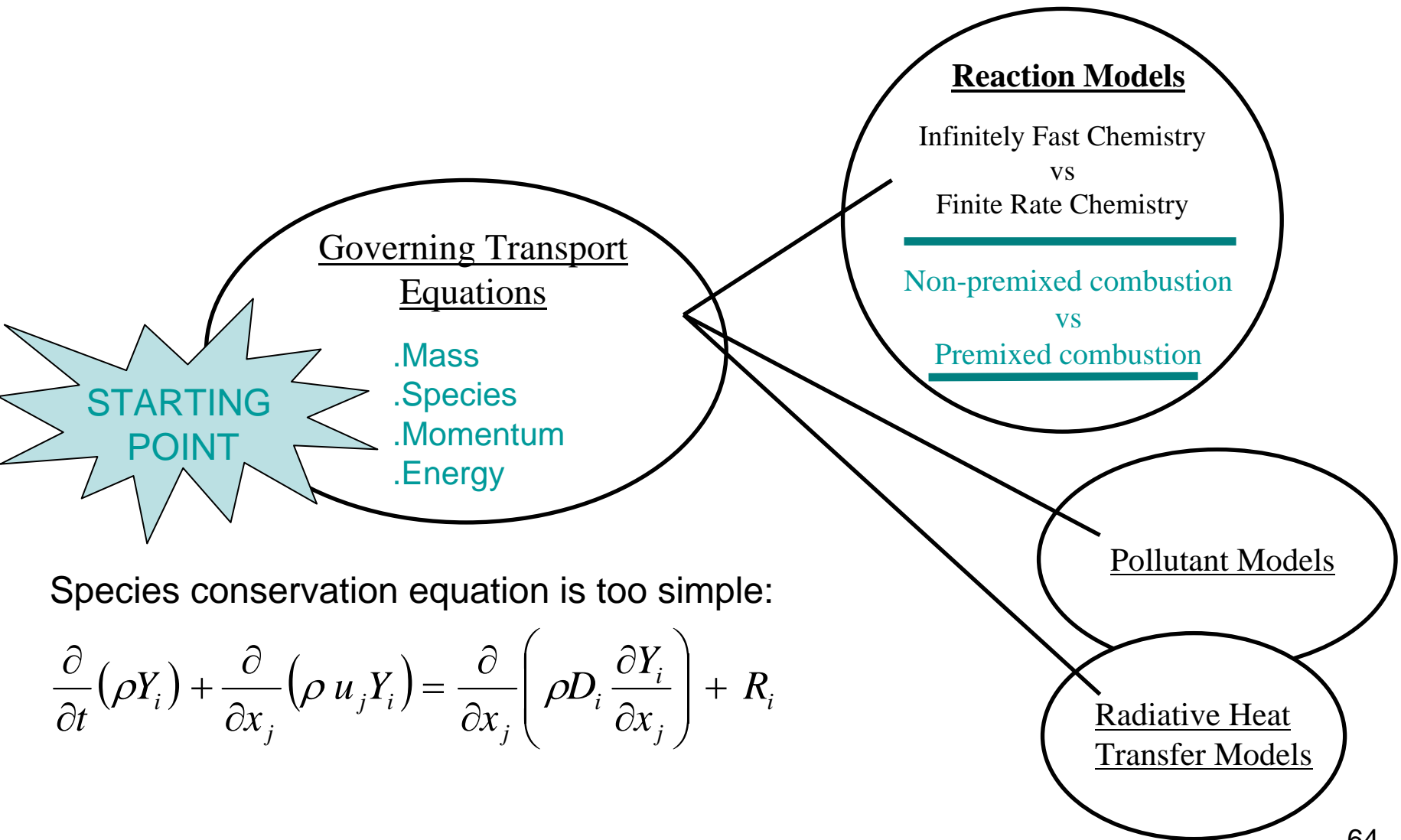


Reasons for modeling and simulation

- Fundamental understanding of the process is possible under correct assumptions
- Sensitivity analysis
- Aid in scaling systems to either larger or smaller throughputs
- Aid in optimization and control strategies



Modeling a Combustion System

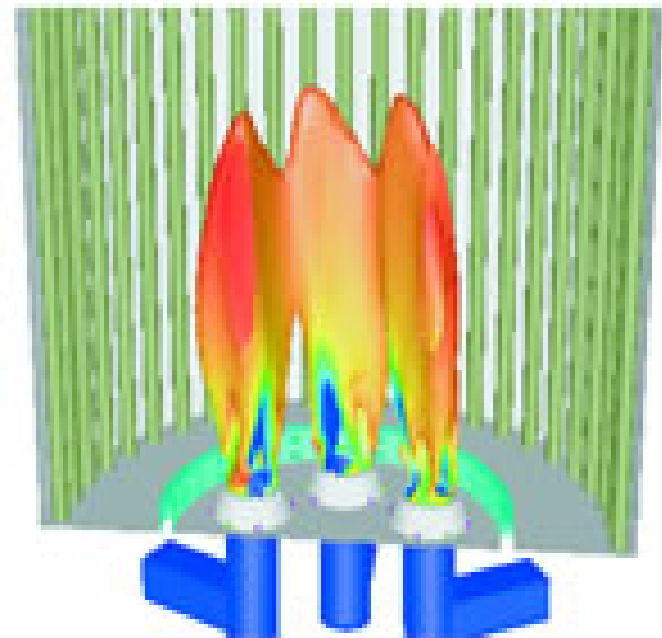


CFD

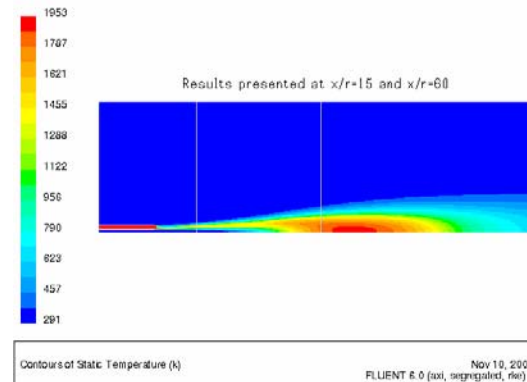
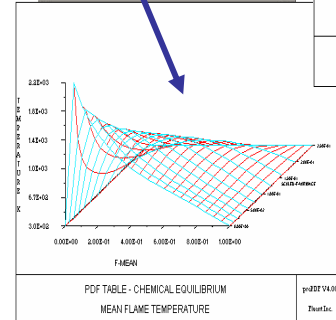
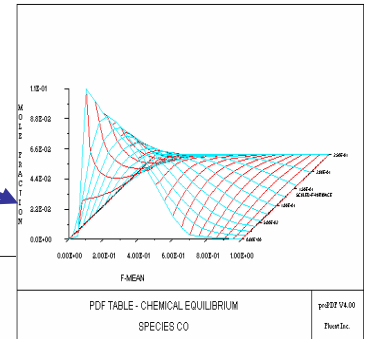
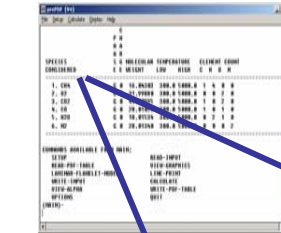
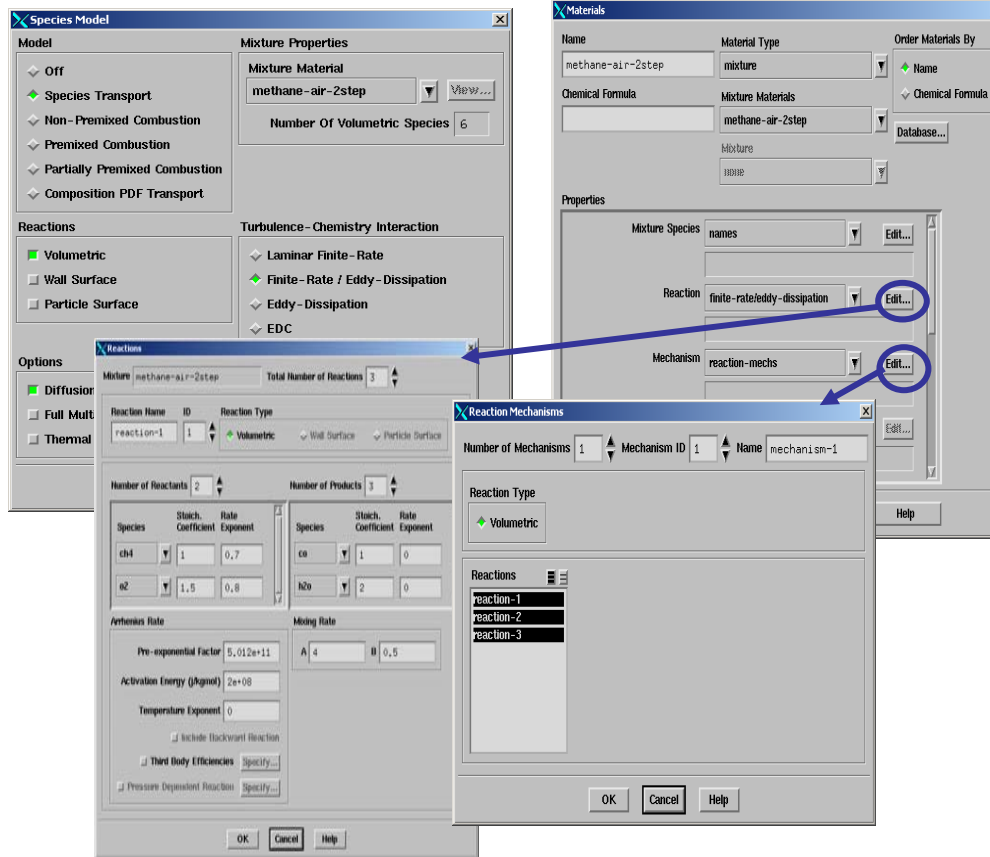
- CFD is a powerful numerical tool for simulating the complicated fluid flow, heat transfer, and chemical reactions in a combustion system
- CFD has gained in popularity in recent years due the dramatic increase in computer power
- CFD is based on fundamental physics and not on empirical functions
- Complexity of the problem requires specialized knowledge to set up complex 3-D CFD simulations and interpret the results

CFD Solution Methodology

- Mesh generation
- Flow specification
- Calculation (numerical solution)
- Analysis of Results



Fluent Capabilities...



Fluent FlowLab

- Reinforce basic concepts of fluid mechanics and heat/mass transfer using computer simulation
- Use computing exercises to augment and complement existing laboratory-based curriculum
- Expand the learning experience with real-world applications of fluid flow and heat/mass transfer
- Provide visualization and interactivity without requiring higher level expertise needed to run Fluent (mesh creation, geometry)

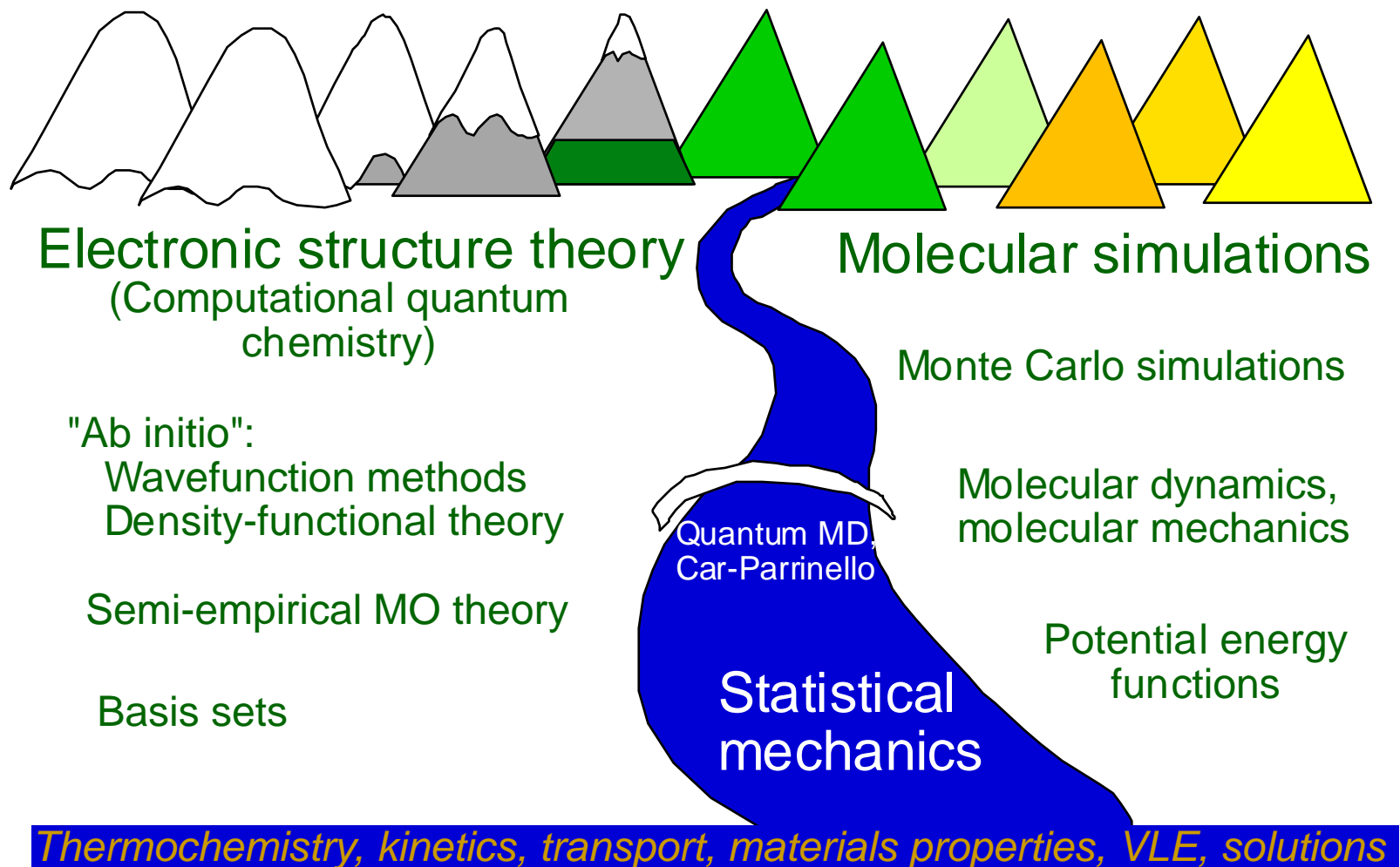
Fluent FlowLab Exercises

- Flow in an orifice meter
- Developing flow in a pipe
- Sudden expansion in a pipe
- Flow over a heated plate
- Flow over a cylinder
- Flow over an airfoil
- Steady state conduction
- Heat conduction in parallel

Product Design and Computing

- Called “reverse engineering” by MEs
- ChEs want to be able to realize specific product properties (e.g., a polymer) through design of a processing scheme (market-driven)
- Holy grail of materials design – software that takes desired product properties and determines realistic chemical structures and material morphologies that have these properties
- Molecular modeling and simulation – first principles approach (quantum mechanics)

Molecular and material structure



Reengineering the Curriculum

- PROCEED ÷ Project-Centered Education in Mechanical Engineering – U. Texas
 - Ford and Applied Materials funded remaking the curriculum to produce the “mechanical engineer of the future”
 - Fifteen different curriculum projects carried out since 2000 (14 courses)
 - Hands-on work implemented in instructional labs paired with theory courses.
- Frontiers of Chemical Engineering Workshops (NSF-funded) – 50 ChE departments.

Frontiers of Chemical Engineering Workshops (2003)

(see <http://web.mit.edu/che-curriculum>)

- Changes in science and the marketplace call for extensive changes to the chemical engineering curriculum.
- The enabling sciences are: biology, chemistry, physics, mathematics.
- There is a core set of organizing chemical engineering principles, emphasizing molecular level design.
 - Molecular Transformations, Multi-scale Analysis, Systems
- Chemical engineering contains both product and process design.

Ingredients of the New ChE Curriculum

- The curriculum should integrate all organizing principles and basic supportive sciences throughout the educational sequence.
- All organizing principles should be operative in the curriculum throughout the sequence and should move from simple to complex.
- The curriculum should be consistently infused with relevant and demonstrative laboratory experiences.
- The curriculum should be consistently infused with relevant examples, open-ended problems and case studies.

Systems

- Systems: tools for synthesis, analysis and design of processes, units and collections thereof
- Introduction to Systems (Sophomore)
 - conservation laws for simple dynamic and steady state systems
 - build model for experimental dynamic system
 - collect and analyze lab data
 - build numerical simulation for simple models
 - parameter estimation (exposure to complexity and uncertainty)
 - construct equipment/sensor

- Introduction to Molecular Systems (Junior)
 - stochastic systems and molecular level reactions as systems
 - simulation as an enabling technology
 - use of models in predicting system behavior (analysis) and in shaping system behavior (synthesis)
 - energy and mass integration, design for the environment
 - optimization principles for design, parameter estimation and decision-making
 - examples from microelectronics, catalysis, systems biology, stochastic kinetics

- Systems and the Marketplace (Senior)
 - multi-scale systems: separation and resolution of time and length scales
 - design and analysis of feedback
 - monitoring, fault detection and sensitivity analysis
 - design experience: economics/business skills, safety, marketing, environmental impact, life cycle analysis, ethics, globalization, IP
 - process operations
 - planning, scheduling, and supply chains
 - Tie-in with Beaker to Plant (Process and Product Design)

Laboratory Experience

- Includes VLAB, ILAB and hands-on
- Will teach:
 - teamwork and communication skills
 - ability to handle real (i.e., messy) problems and data
 - open-ended problem-solving
 - safety
 - environmental and regulatory issues
 - reinforcement and visualization of concepts from courses
- Can also teach
 - experimental design
 - basic lab techniques and instrumentation

Possible Case Studies

- Desalination of sea water
- Hydrogen from biomass
- Global climate change
- Production, separation, and purification of natural products and recombinant proteins
- Insulin regulation
- Drug patch design
- The human body as a chemical process
- Cell design (human, animal, plant) and regulation of metabolic pathways

Conclusions

- Integration of computing throughout the curriculum is hard work, requiring faculty to give up some independence in order to reach consensus.
- While contentious issues remain, common approaches among departments are growing.
- There will be continued pressure on the number of hours in the curriculum, forcing more integration of computing skills into core courses (vs. more courses devoted to computing).

- The number of software tools to be mastered by students should be minimized.
- Courses on fluid mechanics, heat transfer, and thermodynamics offer new possibilities for introduction of computing physical and chemical behavior.
- More interdisciplinary cooperation should be pursued for teaching courses in statistics, computer software tools, and numerical methods.

GAMS Newsletter Number 16

Bruce McCarl

GAMS 21.4 release

GAMS Development Corporation has recently released version 21.4. Version 21.4 expands some language capabilities. Release notes are on the GAMS web site at <http://www.gams.com/docs/release/release.htm#21.4> . Some of the new features within this release are discussed below. The software can be downloaded from <http://www.gams.com/download/> .

Speed Enhancements

Execution time characteristics have been improved. In particular, as discussed in the Execution speed chapter of the McCarl Guide GAMS statements can execute unnecessarily slowly if one is not careful about index ordering. For example $x(i,j,k)=y(k,j,i)$ can be slower than $x(i,j,k)=y(i,j,k)$ for exactly the same contents of y just different index ordering. Version 21.4 has features to speed up execution in such cases with the release notes showing 90% reductions in execution time. Work has also been done on speeding up lead and lag operators.

GAMS use of these speedups (that involve automatic reordering of data arrays during execution) is controlled by the command line parameter `sys11`, where by default GAMS uses the new procedures but if the user sets `sys11=1` GAMS reverts to the old procedures.

Solvers

Solver capability upgrades, solver availability and pricing developments are present.

- BARON, CONOPT, MINOS, OQNLP and XPRESS have new features.
- NLPEC and PATHNLP are upgraded from beta versions.
- New solvers are contained
- GAMS/COINGLPK and GAMS/COINSBB, two free LP/MIP solvers from the Free Computational Infrastructure Operations Research (COIN-OR) Initiative.
- MSNLP a stochastic search algorithm from Optimal Methods, Inc for global optimization problems.
- A pricing discount is available for those purchasing at least two of the global solvers BARON, LGO, or MSNLP, amounting to 25%. Package discounts are also present regarding the solvers CONOPT, MINOS, and SNOPT. See the sales page for details.

McCarl User Guide

The release contains the newest version of the McCarl GAMS user guide current through GAMS 21.3. This is now automatically installed by the Windows installation procedure.

Unfortunately the current release is missing the document chapter Variables, Equations, Models and Solves. For now this can be fixed by going to the web and downloading that chapter then placing it in the subdirectory.\docs\bigdocs\gams2002 of your GAMS system which on my machine is C:\Program Files\GAMS21.4\docs\bigdocs\gams2002. A soon to arrive maintenance release will fix this.

Other features

The release notes indicate 21.4 also contains

- New entries in the model and test model libraries that illustrate new features.
- Procedures to rank order data in parameters (GDXRANK) as documented here.
- IDE features regarding licenses.
- New functions regarding time of day, execution time, execution error codes, beta distributions and gamma distributions.
- Features that enable the use of embedded values in parameter and set data statements.
- Suffixes Grad and Hess that get exact point derivatives from any function.
- Procedures to reformat dates and insert tabs in put files.
- An option suppressing the logging of put files.
- A \$IF option that allows testing for the solver being used at compile time:\$IF SOLVER command
- \$if NOT solver baron \$goto nobaron
- Improved underflow control.

GDX, Timing of \$ commands versus EXECUTE_UNLOAD

When one is using \$ commands in column 1 of a GAMS program (not \$ conditionals) one must remember that the only data available to the commands is that in the set or parameter statements not any of the data developed by program execution. Consider the example

```
Set          i          /a1,a2,a3,a4/;
Parameter    x(i)       /a1 2,a4 12/;
x(i)$ (x(i)=0)=5;
$gdxout ss.gdx
$unload x
$gdxout
execute_unload "ss1.gdx" x
```

In this example the files ss.gdx has 2 entries for x while the file ss1.gdx has 4 entries. Why because the \$ commands are all executed at compile time and the statement redefining x will not be performed until execution time.

\$UNLOAD, and \$CALL GDXRW or any other form of \$CALL can never use data computed during the GAMS run. If one wishes to use such data then

EXECUTE_UNLOAD and EXECUTE GDXXRW must be used. I think use of \$UNLOAD and \$CALL GDXXRW should be avoided if at all possible. The McCarl guide available through the web or the IDE on Windows machines elaborates in the chapters on GDX file usage, and Links to Other Programs.

Transferring data via TXT and GDX files

Erwin Kalvelagen has recently created programs that will pass information to and from TXT files at time of program execution. These are open source programs called gdx2txt.exe and txt2gdx.exe described in Erwin's webpage at <http://www.gams.com/~erwin/> through Interfacing GAMS with other applications (<http://www.gams.com/~erwin/interface/interface.html>): Tutorial and examples specifically in the section on the GDX API under language bindings and are available for download through that document. These permit data exchange with user written programs. Consider the following suggestive example:

```
Set      i      /a1,a2,a3,a4/;
Parameter  x(i)  /a1 2,a4 12/;
alias(i,j);
parameter y(i,j);
parameter z(i,j);
x(i)$ (x(i)=0)=5;
execute_unload "ss1.gdx" x;
execute "gdx2txt.exe in=ss1.gdx id=x out=mytext.txt"
y(i,j)=ord(i)*ord(j);
execute_unload "ss1.gdx" y;
execute "gdx2txt.exe in=ss1.gdx id=y out=mytext2.txt"
execute "del mytext3.txt";
execute "copy mytext2.txt mytext3.txt";
*execute "myfavoriteprogram.exe";
execute "txt2gdx.exe out=ss1.gdx parameter id=z in=mytext3.txt";
execute_load "ss1.gdx" z;
display z;
```

Herein the file mytext.txt will contain the data for the parameter x in a file looking as follows

```
i1 2
i2 5
i3 5
i4 12
```

while the first 6 lines of mytext2.txt contain the information for the two dimensional parameter y

```
i1,j1 1
```

i1.j2 2
i1.j3 3
i1.j4 4
i2.j1 2
i2.j2 4

finally the entries in the GAMS parameter z at the end of the program is the information ultimately in y but after

- unloading it to a GDX
- then moving it to a text file
- then copying it to another text file
- then loading to a GDX file
- then bringing it back into GAMS.

Here one could replace the copy command with an Execute that runs of a user written program that reads the TXT file passed from GAMS then creates a TXT file for passage back to GAMS. The formatting requirements for such files involve using set names consistent with the GAMS program then for multidimensional items separating the various set elements with periods.

Courses offered

I teach Basic GAMS in College Station Nov 30-Dec 3, 2004. An Advanced GAMS class will be offered January 4-7, 2005. Further information and other courses are listed on <http://www.gams.com/courses.htm>.

GAMS Newsletter Number 17

Bruce McCarl

GAMS 21.5 release

GAMS Corporation just released version 21.5 which expands some language capabilities and includes new solver libraries for several solvers. It also includes the new interior-point NLP solver KNITRO. Release notes are available on the GAMS web site at <http://www.gams.com/docs/release/release.htm#21.5>. Some of the new features within this release are discussed below. The software can be downloaded from <http://www.gams.com/download/>.

Speed Issues

As discussed in the last newsletter GAMS, has been working on execution speed. Under some circumstances (generally involving leads and lags and index ordering) version 21.4 had some difficulties and version 21.5 corrects those.

I recently discovered a major speed enhancement that when tested can reduce execution speeds for minutes to under a second for certain types of slow statements. In particular, suppose I want to define a parameter that contains sums of numbers within a more complex parameter where the numbers involved are drawn from the middle of the more complex item. For example,

$$Z(I,L,N)=\text{sum}((K,J,M), Y(I,J,K,L,M))$$

I have found cases where this can be made much faster by coding it as follows:

```
Z(I,L,N)=0;  
Loop((I,J,K,L,M)$Y(I,J,K,L,M),  
      Z(I,L,N)= Z(I,L,N)+Y(I,J,K,L,M));
```

Naturally you should not do this unless you find the statement to be slow using the profile and profiletol options as discussed in the speed chapter of the McCarl User Guide. See <http://www.gams.com/dd/docs/bigdocs/gams2002/speed.pdf>.

Solvers

Solver capability upgrades are present for CONOPT, CPLEX, MOSEK, XA and XPRESS. Also, a new interior point NLP solver, KNITRO, has been introduced. Documentation for KNITRO is available from <http://www.gams.com/solvers/knitro.pdf>.

Put enhancement

A new feature has been added to put files that simplifies adding in several lines of text.

In particular new statements are present that are \$onput and \$offput that results in all the statements in between being placed into the currently active put file. Namely

```
set i /1*2/;
file myput
put myput
loop(i,put 'Before set i ' i.tl /);
put '*****' /
$onput
Hello
this is line 1
this is line 2
$offput
put '*****' /
loop(i,put 'After set i ' put i.tl /);
```

results in the file myput.put that contains

```
Before set i 1
Before set i 2
*****
Hello
this is line 1
this is line 2
*****
After set i 1
After set i 2
```

Note this set of \$ commands differs from all others in GAMS in that they are executed at execution time not at compile time.

Ordering and set elements

Some new features have been entered on set ordering. Namely the universal set is not in a sorted order and can be used with the ord command or set leads and lags. Furthermore a new function SortedUels(*,*) allows one to work with elements in the universal set that correspond to individual elements. I have not worked with this much but it may ease frustration of some who desire to use leads and lags and ord on computed sets. See the example below:

```
set i /1*2/;
set j this set will be regarded by gams as un
ordered /0*6/;
set k(j) this set is computed;
k(j)=yes;
file myput
```

```

put myput
alias(*,u,u1);
display u;
loop(SortedUels(u,j),
  put ' j as an universal set element ' j.tl ' order ' ord(u) /);
put /
loop(j,
  put ' j as an individual set element ' j.tl /);
put /
loop((u,j,u1,k)$(SortedUels(u,j) and SortedUels(u1,k) and ord(u)=ord(u1)),
  put ' element j ' j.tl ' is same in order as element k ' k.tl /);

```

Herein the sets j and k could not have been used with ord but I can use it on corresponding elements in u and u1. Note however that the elements are in sorted order not in the normal order one might expect (j will be 1,2,0,3,4,5,6 naturally but becomes 0,1,2,3,4,5,6 when used in association with the sorted uel order).

Other features

The release notes indicate 21.5 also contains

- * New entries in the model and test model libraries.
- * New functions: sinh, cosh, tanh
- * \$on/offVerbatim commands for use with the GAMS parameter DUMPOPT
- * \$setDDlist that causes GAMS to catch misspelled 'double dash' parameters

Courses offered

I teach Basic GAMS in College Station Nov 30-Dec 3, 2004. An Advanced GAMS class will be offered January 4-7, 2005. Further information and other courses are listed on <http://www.gams.com/courses.htm>.

FOCAPD 2004

Foundations of Computer Aided Process Design

July 11-16, 2004

The Friend Center
Princeton University, New Jersey

<http://www.focapd.org/FOCAPD2004>

The major theme of FOCAPD 2004, Discovery Through Product and Process Design, reflects this remarkable shift in the industrial sector. Princeton University Professor Christodoulos A. Floudas and Dr. Rakesh Agrawal of Air Products and Chemicals, chair this conference with a goal to create an academic and industrial dialogue, a critical assessment of existing enabling technologies, a discussion on research, education, and industrial needs, and a forum of new directions, challenges and opportunities in product and process design.

FOCAPD 2004 will be held at the Friend Center at Princeton University, Princeton, New Jersey, July 11-16, 2004. This international conference will attract world-renowned experts from academia and industry, researchers and practitioners from government laboratories, product and processing industries, technology and consulting companies, and graduate students. Please check out the above website for more information.

Foundations of Systems Biology in Engineering — Overview

The field of systems biology has emerged in the last several years at the interface between genomics and engineering & quantitative sciences—with an overall emphasis of analyzing complexity in biological systems using integrative, systems approaches. The problems addressed in systems biology range from reverse engineering regulatory mechanisms to expand the boundaries of scientific knowledge to forward engineering problems involving drug targeting and the development of biomedical therapies.

FOSBE 2005 (Foundations of Systems Biology in Engineering) is the first in a series of a conferences offered by the CACHE organization to address the emerging challenges in the field of Systems Biology. The conference is unique in that it addresses not only current research problems, but also the curricular developments and industrial needs and challenges in this important intersection of biology and engineering.

FOSBE 2005 will bring together researchers from biochemical engineering, systems engineering, complex systems research, computational biologists, computer science, and experimental biologists. Furthermore, the audience will include academic researchers, experts from industry (including pharmaceutical, biotech, and biomedical products), government laboratories (DOE, and Department of Defense), and federal funding agencies—to discuss the advances, challenges, and emerging opportunities in systems biology.

FOSBE 2005 will offer a keynote presentation, 5 technical sessions and one panel discussion over the course of three days. Breaks and hospitality suites will offer time for informal discussions, demonstrations, and networking. The technical sessions will feature 3 plenary speakers, while the contributed paper session will comprise brief oral presentations and poster presentations.

CHEMICAL PROCESS CONTROL – CPC7

January 8 – 13, 2006

Fairmont Chateau Lake Louise

Assessment of Core Technologies and Emerging Applications

The overall goal of the CPC conference series is to evaluate current progress in the process control field and to identify new intellectual challenges that may have a fundamental impact on future industrial practice. Specific goals of CPC 7 include:

1. Assess the current state of process control theory and practice.
2. Present tutorial overviews for non-specialists in relevant areas of systems and control theory, particularly emerging and new areas.
3. Provide a forum for in-depth discussions between university researchers, industrial practitioners and commercial control technology vendors.
4. Expose practitioners and vendors to significant new tools emerging from the research community to stimulate wider implementation.
5. Present promising research directions for the next decade.
6. Evaluate needs and challenges in the process industries for the next decade.
7. Evaluate opportunities for applications in non-traditional industries.
8. Evaluate the current status of process control education at the undergraduate and graduate levels.

CPC 7 is an international conference attracting participants from North and South America, Europe and the Pacific Rim. Based on previous CPC meetings, approximately 50% of the attendees will be from industry and government with the remaining attendees from academia.

In the tradition of previous CPC conferences, all oral presentations will be invited. Technical sessions will be scheduled in the mornings and the evenings, with afternoons free for skiing, socializing and in-depth discussion. Morning sessions focusing on enabling control technologies will consist of four presentations and a panel discussion. Evening sessions focusing on emerging control applications will consist of three presentations. One afternoon will be devoted to a poster session for contributed papers. Vendor and software displays will be presented on two consecutive afternoons.

FOMMS 2006
FOUNDATIONS OF MOLECULAR MODELING AND SIMULATION

Semiahmoo Resort, WA
July 9-14, 2006

Molecular Modeling and Simulation: Tools for Innovation

FOMMS 2006 is the third international conference showcasing the applications and theory of computational quantum chemistry, molecular science, and engineering simulation. The motivation for this conference is the continual need for precise control of product properties, the accurate prediction of physical properties, and the development of a fundamental understanding of the chemical process that allows the efficient creation of new products that meet specific marketplace demands. Theoretical and algorithmic advances along with modern computing technology routinely lead companies to capture the cash value of truly sustainable, far-reaching competitive advantage. A molecular-level understanding of these chemical processes lead to model mechanisms that are robust, pertinent, scalable, and most importantly, integratable across statistical, chemical, and engineering technologies. The future for these methods is extremely bright as they continue to prove their value to the chemical and chemical-related industries in the coming decade.

Topics of special interest include the following:

- Multiple Time Scale & Mesoscale Methods
- Advances in Modeling & Simulation
- Nanoscience & Nanotechnology
- Biological Applications
- Reaction Engineering
- Electronic Materials
- Polymeric Materials
- Future Vision

FOMMS 2006 is a scientific modeling meeting balanced between molecular simulation and computational chemistry. The format will follow the highly successful FOMMS conferences held in 2000 and 2003. All talks will be invited and will represent state-of-the-art reviews in the particular special topic areas. Two poster sessions will provide opportunities for all attendees to present their work. One afternoon will be devoted to a software/hardware demonstration session for providers to showcase their products and services. In addition, the schedule provides large blocks of time for informal discussions, relaxation, or leisure as well as several receptions to facilitate interaction between conference participants. Each presentation will be rigorously reviewed and edited.

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