Workshop Report

PROCESS MEASUREMENT AND CONTROL: INDUSTRY NEEDS

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Abstract

The purpose of this interim report is to provide a description of the key findings of the workshop, entitled "Process Measurement and Control: Industry Needs," which was held at the Sheraton New Orleans, March 6-8, 1998.

INTRODUCTION

The U.S. chemical industry is among the most successful industries in the United States: Through partnerships and investment, it produces $400 billion of products annually and provides over one million U.S. jobs. Having recorded a trade surplus for forty consecutive years, it is the country's premier exporting industry: Chemical industry exports totaled $60.8 billion in 1995, accounting for more than 10% of all U.S. exports, and generated a trade surplus in excess of $20 billion. The continuing success of the chemical industry is a result of its ability to evolve in response to new technological and societal needs. For example, among industrial and manufacturing groups, it is the leading investor in research and development (over $18 billion in 1995, and responsible for one in every eight patents issued). With the increasing emphasis on specialty chemicals and products for the biomedical and advanced materials industries, the chemical and related processing industries are faced with the need for increasingly precise control of final product properties to meet specific demands.

Two key enabling technologies for the continued success of the chemical industries are chemical measurement and process control.

Manufacturing operations will require a continuous infusion of the newest information and process control technologies if the chemical industry is to maintain its global ability to deliver products that best serve the customer reliably at the lowest cost. To achieve that goal the chemical process industry uses many computer systems that range from process control through equipment monitoring and maintenance to production, planning and scheduling. Today these systems are purchased as stand-alone entities. As the industry works to achieve more efficient and effective operations these software systems will have to become more tightly integrated without becoming unmanageable monolithic systems. Emerging software technology will be needed to solve these problems.

Chemical analysis is a critically important enabling technology essential to every phase of chemical science, product and process development, and manufacturing control. New knowledge and insights about existing and new processes, developed as a result of advances in chemical measurement over the past two decades, have greatly accelerated progress in chemical science, biotechnology, materials science, and process engineering. Chemical measurements also play a key role in numerous related industries, such as pharmaceutical, pulp and paper and food processing. During recent years, impressive advances have been made in the resolution, sensitivity, and specificity of chemical analysis. The conduct of analytical chemistry has been transformed by advances in high-field superconducting magnets, multiple-wavelength lasers, multiplexed array detectors, atomic-force and scanning-tunneling microscopes, nonscanning spectral analysis (for example, Fourier transform), and the integration of computers with instrumentation. The recent extension of these methods to the detection and spectral characterization of molecular structure at the atomic level shows that the ultimate limit of specificity and sensitivity of chemical measurements can actually be reached in tightly specified experiments.

More broadly, the inclusion of analytical specialists as full partners in research teams has been shown to enhance greatly the efficiency of research teams in chemical synthesis, surface science, catalysis, nanostructure science and technology, and environmental chemistry. Improved real-time control and increased process understanding can be achieved with sophisticated analytical instrumentation. However, comprehensive compositional analysis is seldom used in chemical manufacturing process control. The main reasons for this are either the high acquisition and maintenance costs of the instruments or the complexity and skilled personnel requirements of the off-line methods. In many cases real-time analytical measurements are not generally available, either on-line or off-line. Most compositional measurements are still used to provide post-production quality control assessment and demonstrate EPA compliance. Regulations dictate which methods are used for environmental measurements, rather than allowing the application of the best available technology and instrumentation.

Needs and Challenges

The potential for improved operational performance offered by the integration of measurement, control and information systems needs to be exploited to maintain and improve the competitiveness of the U.S. chemical industry. Elements required for improvements in computer capabilities include the following: (i) integrated systems to allow the rapid implementation of new product and process technology globally, (ii) the availability of accurate, current information to support global strategies to enhance company competitiveness, (iii) significant improvements in make-and-deliver systems.

While significant progress has been made in moving process analytical measurements from the laboratory to the manufacturing line, more real-world chemical measurements are still conducted off-line. Most of the more spectacular recent achievements in this area have been made by highly skilled scientists using one-of-a-kind instruments. The isolation of sophisticated methods of chemical analysis from the environments in which they are most needed--ranging from R&D laboratories through manufacturing facilities--is a major limitation in present-day chemical measurements. Both state-of-the-art research-grade instruments and laboratory prototypes often lack the robustness, sophistication, and general utility required for effective, widespread use by nonspecialists.

Through numerous meetings and workshops, other non-technical barriers have also been identified. Among these are:

- Barriers to technology transfer from national laboratories need to be lowered
- Mismatch in time scales between university research and industry needs
- Communication within the industrial community on pre-competitive issues and common measurement and control challenges is poor
- Initial explorations by industry-university teams are impeded by concerns for intellectual property rights

Major Drivers

The major drivers for evolutionary and revolutionary changes in our chemical measurement and control capabilities are:

- Cost reduction, increased efficiency (e.g. via “Just-in-time production”)
- Speed to market requirements
- Product quality improvement (especially critical for global competitiveness)
- Environmental & safety concerns
- Support for innovation leading to new products and processes (e.g. how does a catalyst really work, structure - properties relationships)

Workshop

In recognition of the recent growth and the perceived new opportunities in process measurement and control, a workshop on this topic was held at the Sheraton New Orleans on March 6-8, 1998. Sixteen invited speakers and discussants from academia, industry and national laboratories presented their perspectives on the current state-of-the-art, applications in industry and future needs in various areas of process measurement and control. Thirty additional participants, also representing academia, industry and national laboratories, attended and participated in the workshop. Many of these individuals were invited; however, some were unsolicited applicants who learned of the workshop through colleagues and responded to a web-based call for participation located at the web site **http://udel.edu/~fdoyle/V2020.html**.

The goals of the workshop were five-fold:

1. Identify the current state-of-the-art for process measurement and control, including their current impact on academic and industrial research and development;
2. Project where these methods can be in 25 years, and the expected impact of these methods over that period;
3. Identify the challenges and roadblocks that delay advancements in these technology areas;
4. Identify strategic research investments that might facilitate the achievement of these latter capabilities and ensure their widespread utility to both academic and industrial communities;
5. Produce a report to the research community served by the NSF, NIST, and NIST ATP concerning the findings of 1-4.

A unique feature of this workshop was that chemists and chemical engineers were brought together in a common forum to address the common interests in process measurements for control. Individual breakout groups were comprised of a mixed group from academia, industry, and the government labs. Furthermore, each group was split between measurement scientists and control engineers, and the groups each addressed one control topic and one measurement topic. In this manner, a "single track" was achieved.

In the remainder of this preliminary report, the summary findings of the workshop will be discussed. Several speakers were asked to provide overviews of, and assess the state-of-the-art in, process measurement and control. Others were asked to describe successes of current methods in industry and academia, and to assess needs into the future. This was done around eight topical areas, and the balance of this report is organized around those areas:

- Nonlinear model predictive control
- Performance monitoring
- Estimation and inferential control
- Identification and adaptive control
- Molecular characterizations and separations
- Process sensors
- Microfabricated instrumentation
- Information and data handling

CRITICAL NEEDS, RESEARCH PRIORITIES, AND PATH FORWARD FOR PROCESS MEASUREMENT AND CONTROL

In the following sections, the conclusions of the respective breakout groups are summarized. In each case, the following three issues are addressed: (i) challenges and needs, (ii) research priorities to meet these needs, and (iii) concrete action items to establish a path forward. In the prioritization of research investments, the following notation is adopted to denote the estimated time-scale of those items: **S** - short term (3-5 years), **M** - medium term (6-9 years), and **L** - long term (> 9 years).

Nonlinear Model Predictive Control

Critical Needs and Challenges

Nonlinear model predictive control (NMPC) has found successful application in a limited number of mainly academic example cases to date. These examples are typically low order (less than 20 states), low dimensionality (single-input single-output (SISO) or 2x2), and assume full measurement or full state observability. In the discussion, a number of issues were raised with regard to the components of nonlinear MPC, and the following challenges were identified:

1. There is a need for an analysis tool to determine the appropriate technology to use in a model-based control application. Such a tool would require as input: a process description, a performance objective, and the definition of the operating region. For example, when would NMPC yield significant advantages over MPC in an industrial application?
2. Is there a more efficient way to represent complex physical systems so that they are more amenable to optimization based control methods?
3. Development of improved customizable optimization techniques is needed to handle the rigorous demands imposed by increasingly complex nonlinear models.

Research Investments Required to Meet Critical Needs

In summarizing the discussion, the following general need was identified: "*Development of practical nonlinear model-based control techniques with quantifiable plant performance improvements that can be supported in an industrial environment*." More specific recommendations follow.

Development of improved modeling paradigms that exploit process data, and various forms of prior knowledge [S,M]

- Address issues in fundamental modeling of large-scale complex processes:
  - model reduction techniques relevant to NMPC
  - low-order physical modeling approaches
  - address the support and maintenance issues of complex models
  - try to understand if and how various common model attributes contribute pathological features to the corresponding optimization problem (for example: a non-smooth error surface)

- Hybrid modeling: develop new methodology for effective combining fundamental and empirical modeling techniques.
- New approaches for nonlinear empirical model development:
  - input sequence design (length, excitation, plant-friendly)
  - identify model structures that capture process behavior, are amenable to optimization-based control, and admit analysis
  - develop methods that allow adaptation for nonlinearly parameterized models

Algorithm engineering approaches to tailored solutions for optimization-based control [S,M,L]

- Improve large scale optimization methods for plant-wide applications.
- Develop improved optimization algorithms for nonconvex optimization problems.
- Develop hierarchical solution methodologies that exploit problem structure.
- Explore more efficient use of computer time: *e.g.*, when convergence occurs before the controller update use "surplus time" to precompute some parts of the next step.
- Can a warm-start initialization of optimization be used during the MPC update step?

Develop characterization tools for process nonlinearity that yield control-relevant information [S,M,L]

- Determine the appropriate input set for characterization of process nonlinearity (operating regime, process model, performance objective, control structure).
- Develop a suitable mathematical metric for performance to be used in characterization of benefit.
- Map control technology to process characterization.

Long term maintenance and support of the NMPC algorithm in an industrial application [M,L]

- Develop a component-based toolkit for synthesis.
- Development of support tools for long term on-site maintenance:
  - performance assessment (*e.g.*, fault detection)
  - identification
  - performance interpretation (*e.g.*, fault diagnosis)
  - control tuning: *e.g.*, develop intuitive simplified set of tuning parameters that combine several of the existing parameters (horizon lengths, weights, *etc.*)

How to Get There

Establish collaborations and communication between scientists and engineers in the measurements and controls area:

- interdisciplinary workshops (such as the present one)
- within and among consortia
- involve vendor community in above activities

Enhance contacts between control and optimization communities:

- exchange speakers at professional and consortia meetings
- involve the vendor community

Introduce curricular changes:

- short courses to teach the NMPC technology

Establish CAPE-OPEN like initiative in the control technology area to ensure standardization, long term maintenance, and technology deployment.

Establish industrial challenge problems with complete description and performance metrics.

Estimation and Inferential Control

Critical Needs and Challenges

1. To measure critical product quality variables (the basis for selling products) that are currently difficult or impossible to measure; and incorporate into control strategies.
2. To improve theory underlying parameter/state estimation (especially concerning convergence for nonlinear systems).
3. To reformulate the problem to take into account varying levels of available data granularity:
   - Granularity in time; geographical location; frequency; degree of information
   - Reformulation should be flexible enough to to handle changes in such granularity.
4. To quantify adequacy of inferential models
   - When is the model/estimate good enough?
5. To make possible the broad use of hybrid modeling approaches (systematic combination of the data-driven and the knowledge-driven approaches).

Research Investments Required to Meet Critical Needs

To develop a framework for hybrid modeling (combination of “data-driven” and “knowledge-driven” techniques for model development) [M]

To develop tools for determining optimal sensor location. [S]
- Optimal in the sense of providing high leverage on process controllability

To develop controller design methodology that appropriately incorporates different levels of granularity in measurement. [M/L]
- Pressure, temperature, level, flow
- Composition
- Product Quality (including end-user performance properties)

To develop improved state and parameter estimation paradigms and methodologies. [M]

To develop techniques for large-scale modeling. [L]
- Parameter estimation/model calibration
- On-line implementation
- Appropriate reduction in model complexity

To develop techniques for model fusion for consistency of elements. [L]

How to Get There

Industrial challenge problems in Inferential Control developed and broadly circulated;

- Academic response
- Metric for evaluation and framework for providing feedback

Encourage communications between chemists and chemical engineers in appropriate multidisciplinary teams and groups.

Performance Monitoring

Critical Needs and Challenges

1. Communication is needed between levels with different time scale and objectives (e.g. plant-wide vs. process decisions) - vertical and horizontal cultural differences between manufacturing, management, R&D.
2. Problem solutions do not always involve selection of the best technology. Rather, an individual often selects technology based on familiarity.
3. Continuing education of plant personnel does not match the newest technologies and is not uniformly available.
4. Many real situations cannot be managed with first principles or empirical models - a mix is often required.
5. Current industrial monitoring and control systems are limited to simple cases. Expansion to multi-variable, multi-loop, nonlinear, constrained, large-scale, time-varying systems is needed for practical applications.

Research Investments Required to Meet Critical Needs

Assessment of plant-wide variability with full understanding of interaction between the model and the controller. [S]

Root cause diagnosis to find the main cause of the problem for the complete process area. [M]

Development of knowledge-based control and measurement tools. [L]

Develop alternative tuning methods - stochastic versus deterministic responses. [L]

Develop locally automated high performance sensors, transmitters and valves. [L]

Develop methods to address robustness. [L]

In collaboration with industry develop tools to diagnose faults in real systems. [L]

How to Get There

Short courses, workshops

- interactive instruction
- exercises

Development of industrial challenge problems. Teams representing interdisciplinary groups should address these industrial/practical problem solution.

Establish test-bed centers for integrated advanced control systems.

Lower barriers in academia to enable chemists to take chemical engineering courses (math standards barriers).

Expansion of Industry/university cooperative research centers to involve control vendors in industry/academic cooperative centers. Distributed research involving multiple academic institutions can provide the best approach.

Organizers of topical conferences should include chemists and chemical engineers (for example, include chemists in CPC or chemical engineers in IFPAC) and also encourage vendor participation.

Identification and Adaptive Control

Critical Needs and Challenges

For the chemical industry the benefits from improved process control and measurements are estimated to be in the billions of dollars per year. Half of the advanced control strategies that will lead to these benefits are estimated to be dependent on improved measurements.

Most chemical plants are inherently nonlinear and rarely run at steady state. To meet environmental restrictions and conserve energy new plant designs will be much more complex. This leads to more complex process control solutions. This will require us to use more advanced methods of process control to reduce the cost of our capital assets over their entire life.

The following specific challenges were identified:

1. Societal requirements force us to operate more safely, environmentally friendly, and to meet our responsible care responsibilities.
2. A significant driver in the chemical industry is to maximize the capital asset lifecycle.
3. We need to provide process controls to plants that have operating characteristics that change over time. This includes catalyst deactivation, heat transfer fouling, etc.

4. Process modeling is a well established technology that provides value in process engineering and process control. First principle models are not always available, especially for new plants. Therefore, once the plant is running we need to have methods to identify models from plant data for advanced process control.
5. To develop these new capabilities requires greater integration of expertise from various fields, such as, process control, computer science, process engineering, plant engineering, and measurement sciences.

Research Investments Required to Meet Critical Needs

Develop practical adaptive control theory so it can be used in industry. [M]

Develop an approach to use existing first principle process knowledge where possible to integrate identification with adaptive control. [M]

Develop an approach to incorporate advanced on-line process measurement into identification and adaptive control. [S]

Develop improved methods for measurement and adaptive control of batch processes. [M]

Create a practical, unified, and generally accepted fundamental approach to identification and adaptive control. [L]

Develop an approach to integrate advances from computer science, e.g., data mining, database technology, communications, human factors. [M]

How to Get There

Establish meaningful collaboration between measurement and control communities.

Create efficient technology transfer mechanisms from academia to industry.

Create industrial challenge problems with a clearly defined objective and a means for its assessment.

Create on-going and current multidisciplinary continuing education.

Include the vendors to define the component deliver modular systems both in hardware and software. We need to define the components and the interfaces between them.

Molecular Characterization and Separation

Critical Needs and Challenges

Classical molecular characterization and separation technology such as process spectroscopy and chromatography are the current workhorses of process analytical chemistry. While the optimum implementation of process analyzers in 2020 will most likely involve new tools, these techniques will continue to play a large role, especially in the near and intermediate future. Challenges and needs identified for this technology area apply also to the broader class of sensors and information handling.

1. Move laboratory detection limits to process analyzers.

In general, "non-routine" analytical techniques currently run in central laboratories represents the limits of our quantitative confirmed knowledge of the process. This information is obtained by manual sampling and extensive use of highly paid professionals and capital and time intensive analytical methods. As these techniques are applied, we learn more about what is critical for optimization of process operation. For instance, these techniques are used to provide quantitative and qualitative information on catalyst poisons. Once a poison is identified, a process measurement is needed to provide control and monitoring of the catalyst activity in the process. Generally, this requires increased sensitivity and improved precision of measurement. Extension of current laboratory capabilities to process analyzers will increase substantially the degree of process understanding that can be obtained by enabling much more detailed characterization of process dynamics.

2. Implement multidimensional sensors in process applications.

A key strategy used in laboratory instrumentation to increase the amount of information in a single sample run to apply multidimensional or hyphenated techniques (e.g. GC/MS). This approach can be used in plant laboratories today, but commercial process analyzers using this approach are not reliable enough for widespread use.

3. Provide critical information for control of processes involving complex samples such as solids, slurries, and other multiphase samples.

Current process analyzer technology often offers multiple choices for compositional analysis of single phase gas and liquid samples. However, many chemical processes involve streams that are not so easy to handle. Current technology does not offer a broad range of approaches for solids, slurries or other multiphase samples.

4. Provide critical information for control of polymer processes.

A large part of the chemical industry involves production of polymer or processing polymers into formulations or shapes. The product properties that are obtained depend in detail on the structure and composition of the polymer. Currently full description of the structure and composition is difficult and time consuming in the laboratory. Since this information is so difficult to obtain, polymer processes are now controlled using primarily empirical correlations. In addition, industry standard quality indices are based on old technology, and usually don't accurately reflect either polymer structure or customer needs. Today, laboratory methods are available that can provide a detailed description of the polymer structure, which can then be used to develop structure/property relationships for the system. However, these techniques are complex, difficult, and time consuming enough that this is not always done. Even when these structure/property relationships have been determined, and potential control measurements identified, technology to reliably perform these measurements in a process environment is often not commercially available.

5. Provide needed measurements for control of processes based on new process technology, such as the use of biotech based processes for production of specialty or commodity chemicals.

The chemical industry is constantly searching for new approaches to production of products. For example, many chemical companies are exploring catalytic processes based on enzyme catalysts and fermentation based production of chemicals. These new processes will raise new challenges, in the laboratory and especially in measurements for process control.

6. Lowered resistance to implementation of analyzer systems by plant operating personnel.

Engineers and operators at chemical plants have a jaundiced view of analyzers. Sometimes instead of recognizing the potential value that the additional information might bring, they become concerned with the potential problems that come with analyzers. As chemical companies deal with competitive pressures by reducing the number of engineers, mechanics, and operators at typical plants, systems like analyzers that can add substantially to maintenance loads are looked at with increasing suspicion. Current analyzer systems often involve complicated application specific sample systems that are known to be reliability issues and sophisticated instrumentation that requires specialized training for effective maintenance and support.

7. Suppliers are now concerned that they cannot make money in providing improved products to the industry (hardware and software).

Chemical companies often identify new needs for process measurement and get little response from vendors. Most of the vendors serving the analyzer and analyzer systems market are relatively small companies that cannot afford large development investments without assurances of a large market. At the same time, chemical companies find it difficult to share information about process technology that would allow definition of common problems with larger market potential.

8. Optimize placement of sensors and analyzers to provide greatest leverage on the control of the process.

What an analyzer measures, how well it measures it, where it measures it, and how it is used by the control system all have an effect on the overall effectiveness of the control system. Today, intuition, empirical knowledge, or accident have the strongest impact on determining these factors. Improved communication and understanding between analytical chemists and engineers could impact this, as well as the development of appropriate modeling technology.

9. Extract the maximum amount of information from the measurement system, and turning that information to process knowledge and process control actions.

Measurement systems comprising analyzers and temperature, pressure, level and flow sensors produce a large amount of data. Today we often only use the most obvious data as information (e.g. specific compositions, pressures or temperatures). If the data for a unit operation, or perhaps an entire process were looked at as a whole, much more information about the process might be able to be extracted and turned into knowledge.

Research Investments Required to Meet Critical Needs

Develop analyzers that move current laboratory capabilities to the process, but are robust and easy to maintain and support. [S] (Responds to needs 1 and 2)

- Develop improved analyzers based on molecular spectroscopy.
- Develop faster analyzers based on separations technology.
- Develop analyzers based on use of multidimensional analytical techniques now used in the laboratory (e.g. GC/MS).
- Develop analyzers based on technology not currently broadly used in the laboratory (e.g. microwave, acoustics, dielectric relaxation).

Develop mobile analyzer systems for acquisition of improved fundamental understanding and basic data. [S] (Responds to needs 1 and 2)

Develop technology for characterization of polymers (MW, MWD, branching, etc.) that is amenable to process analyzers for support of control systems. [M] (Responds to need 4)

Develop improved structure/property/processing modeling capability, especially for macromolecular products. [M] (Responds to need 4)

Develop improved technology for physical and chemical characterization of solids and slurries. [M] (Responds to need 3)

Develop needed technology for on-line characterization of new processes used in the chemical industry, such as biotech based processes. [M] (Responds to need 5)

Develop technology that improves the effectiveness of the measurement system in implementing the control strategy. [M] (Responds to needs 8 and 9)

- Modeling technology that enables optimum selection of sampling points and measurement objectives.
- Modeling technology that extracts maximum information from the ensemble of sensor systems.

Develop new approaches to sampling and sample interfaces: [S] (Responds to need 6)

- Assure representative samples regardless of sample size.
- Reliable degassing and debubbling of liquid samples.
- Sample conditioning by various techniques (membranes, distillation, etc.).

Develop analyzer/sensor systems which have low maintenance requirements and are self calibrating and self-diagnostic. [S] (Responds to 6)

How to Get There

Strengthen chemical industry - university ties focused on developing new process analytical chemistry technology.

Provide substantially increased funding for centers and projects that involve partnerships between chemical companies and universities. Provide support for faculty visits and sabbaticals at industrial sites, particularly for analytical chemistry faculty, and support for chemists in industry to visit universities for extended periods of time. Encourage industry co-ops for undergraduate and graduate chemistry students.

Provide improved preparation for new employees and better continuing education for current employees.

Assemble industry group to define skill based definition of expectations of chemists and engineers at all levels. Use this definition to stimulate funding of curriculum development by government agencies and universities.

Establish research facilities to address more straightforward problems, which may not be dissertation level material, but are badly needed by industry (*e.g.*, sampling systems, improvement of simple analyzers).

Hold Vision 2020 Workshop on Process Measurements aimed at involving and getting input from the vendor community.

Sensors

Critical Needs and Challenges

Chemical engineers and scientists have a different concept of sensors. They agree on many common features, such as, accuracy, timeliness, and specific properties either chemical or physical. They agree sensors need to be rugged, precise, and accurate. The chemical engineers' requirement is broader because the requirement for process control is input to the plant automation system. From the chemical engineering perspective all measurement devices are sensors. The measurement specialist tends to qualify measurement devices into several categories. Classically a sensor is a zeroth order measurement device. For this topic area we will define sensors to be zeroth order measurement devices. Another group is responsible for higher order measurement devices (microinstruments). For the chemical industry the benefits from improved process control and measurements are estimated to be in the billions of dollars per year. Half of this stake is estimated to be dependent on improved measurements.

The following challenges were identified:

1. To develop individual sensor systems that are cost effective in any scale process.
2. Societal requirements force us to operate more safely, environmentally friendly, and to meet our responsible care responsibilities.
3. A significant driver in the chemical industry is to maximize the capital asset lifecycle.
4. This requires a broader set of capabilities in our suite of sensor systems to allow us to deal with the more difficult control problems needed to run our plants harder and closer to constraints.
5. To develop these new capabilities requires greater integration of expertise from various fields, such as, process control, measurement technology, computer science, process engineering, plant engineering, statistics, and material science, to name a few.

The technology that is becoming available in this field will cause a paradigm shift in the way we do process control. Therefore attention must be given at all levels to improve interdisciplinary education in chemical engineering and chemistry and training of the current workforce.

Research Investments Required to Meet Critical Needs

Develop easier calibration models and calibration transfer among multiple like sensors and from the laboratory to plant, and from plant to plant. [M]

Develop new transfer functions to allow one to calibrate individual sensor with performance properties and/or process parameters. [M]

Develop methods including sensor data fusion to determine customer product performance properties from multiple process measurements. [M]

Develop technology to provide smart sensors for all process measurements. [M]

- Smart sensors detect faults, are self-calibrating, etc.
- This improves reliability and workforce productivity

Develop systematic approach for new sensor materials. [L]

Develop sensors for multiphase systems. [M]

Develop sensors for solids. [L]

Develop methods to provide low cost sensing strategies. [M]

How to Get There

Define the components and the interfaces between and include vendors in this activity. Induce the vendors to deliver hardware and software that is modular and architecturally open in nature.

Provide a mechanism that enables key participants (National Laboratories, academia, vendors, industrial practitioners) to deliver measurement technology.

Provide user friendly instruments to eliminate the need for a measurement specialist.

Provide new directions in education.

Fund more sensor development, particularly for robust low-maintenance sensors.

Integrate process modeling and information technologies.

Microfabricated Instrumentation Systems

Critical Needs and Challenges

Over the course of the discussion, the following critical needs were identified:

1. Development of low-cost fabrication techniques for micro-scale instrumentation.
2. To define the potential impact of microfabricated instrumentation on process modeling, monitoring, and control.
3. Identification of promising microfabricated technologies, including gas phase analysis and measurement.
4. Develop/fabricate systems that address the following specific challenges:
   - sampling
   - reliability/maintenance/standardization
   - optimal size/cost/bandwidth

Research Investments Required to Meet Critical Needs

In summarizing the discussion, the following general need was identified: "*Enable the design of microfabricated instrumentation systems that address critical needs in process measurement for modeling and control*". More specific recommendations follow.

Identification of appropriate technology that benefits from microfabricated instrumentation. [S,M,L]

- Supplant existing lab technology with microinstrumentation
- Match tools to product property needs
- Develop appropriate metric to optimize the size, bandwidth, and cost of microinstruments
- Match tools to control needs:
  - location and distribution
  - estimation of parameters and unmeasured states
  - reconciliation of data versus model (on-line, calibration)
  - redundancy: sensor fusion

Develop system interlinks to interface the technology with the process and communicate with the control system. [S,M,L]

- physical sampling issues:
  - fouling and plugging
  - statistical representation
  - lag times of sample equilibration versus instrument response
  - quantitative description of device dynamics for model based control
- data reduction and information extraction
- electronic communication and fieldbus issues

Determine impact of microinstrumentation on process modeling, optimization, and diagnosis. [M,L]

- More complex models required due to increased measurement data input
- Address distributed nature (spatially) of new data information in process algorithms

- Develop metrics for screening tools for sensor selection
- Address issues in large scale model-based optimization

Establish reliability to gain acceptance of microinstrumentation for process applications. [M,L]

- Develop new materials and fabrication technology for devices
  - physical structure
  - analyte selective interfaces
- Develop devices to minimize maintenance: including self-diagnostics, fault detection, minimized service requirements, and the capability for in-situ standardization and calibration

Develop complete micro-scale sensing-control-actuation systems [M,L]

- Develop microreactor for pilot-scale studies, novel reaction engineering, and process diagnostics
- Develop hierarchical control systems using micro-sensors-effectors pairs as components

How to Get There

Establish collaborations and communication between scientists and engineers in the measurements and controls area

- interdisciplinary workshops (such as present one)
- within and among consortia
- involve vendor community in above activities

Introduce curricular changes to address new issues raised with microinstrumentation

- short courses
- statistics component in analytical chemistry
- measurement device issues in chemical process control

Information and Data Handling

Critical Needs and Challenges

1. At this time, major academic funding in the field of data handling/chemometrics is from industry, and this funding supports the development of *applications*, rather than *theory*. Specifically, there is a severe shortage of government-based data handling/chemometrics research funding for young scientists working in the area of applied analysis, who will be needed to provide future leadership in the field of data handling.
2. There is currently an alarming shortage of academic chemometricians in the U.S., who will be needed to train the future "implementers" that will transfer this profitable technology to the chemical industry. This shortage will only be increased by the future retirement of several prominent academic chemometricians.
3. Although chemometric methods have been well-proven in selected academic and industrial research environments, they often suffer from a lack of acceptance within Chemistry, Chemical Engineering, and Statistics disciplines. This is very unfortunate, because these areas stand to contribute much to the

further development and implementation of the technology. This situation could be, in part, due to the relatively limited mathematics and statistics backgrounds of physical scientists.

4. A wealth of learning and information regarding multivariate data handling techniques has been accumulated over a wide range of fields (from psychology to geology to astronomy), and a lack of multidisciplinary communication has prevented much of this learning to be applied to the chemical industry.
5. "End-users" and "stakeholders" of chemometric methods in the more-conservative manufacturing environments are skeptical of the technology, and are often unwilling to take the necessary risks to use the technology, despite it's widespread success in more research-oriented environments. This could be caused by both a lack of understanding of the technology and a lack of "ownership" in the technology.
6. There are several vendors that offer packages for calibration and modeling, but the "tools" that are offered for method implementation, validation, maintenance and diagnostics are very limited. This has often meant that the user has been required to develop their own software to properly and safely implement the technology.
7. For those few industrial applications that have been attempted, many have been limited in their profitability by calibration maintenance and transfer issues.
8. The size of the possible chemometrics market is somewhat limited and *very* diversified, and this results in the reluctance of software vendors to develop technology at a price acceptable to the users.
9. Recent downsizing in the U.S. chemical industry has resulted in a serious personnel shortage at all levels of the industry. This situation limits both the ability to conduct focused, applied industrial research in chemometrics, as well as the ability to effectively transfer the technology to manufacturing areas.

Research Investments Required to Meet Critical Needs

Improve calibration transfer capabilities. [S]

Develop tools for implementation. [S]

Develop calibration diagnostics and maintenance tools. [S]

Develop a modular, hierarchical, user-friendly application software interface. [M]

Develop more "interactive" algorithms that incorporate prior knowledge in modeling. [M]

Develop theory of higher order methods. [L]

Develop the theory behind PLS. [L]

Investigate non-stationary, non-linear modeling techniques. [L]

How to Get There

Multivariate data handling education needs to be focussed on a variety of audiences.

- End-users/stakeholders (which include industrial chemists, engineers, lab technicians and plant workers) need to develop a basic understanding of the technology- through short-courses and workshops, for example.
- In addition, education reform at the undergraduate and graduate levels is needed to increase statistical and mathematical expertise of future chemists and chemical engineers in the chemical industry.
- The accreditation of chemometrics courses (ABET, ACS) would go a long way towards this goal.

Chemometrics needs to be more-extensively exposed at some of the "broader-based" technical meetings, such as the ACS national and regional meetings.

A stronger "drive" towards standardization of the technology is also needed, in the form of standard reference data sets and standardized methods and algorithms.

- The ASTM Subcommittee E-13.11 on Chemometrics is currently addressing these issues.

Software for various chemometric algorithms should be made easy to download from the World-Wide-Web, enabling potential users to easily evaluate the wide range of existing and new methodologies for their specific problems.

Software vendors should be encouraged to continue the developments and improvements of their application interfaces that were evident at the PITTCON '98 exposition.

Challenge problems, such as NIST's ANOVA Challenge Problem, need to be designed to rigorously evaluate new and existing chemometric algorithms. Such challenge problems should be formulated such that they "push" the abilities of the techniques and help define the limitations of the techniques.

The identification of additional markets for chemometric methods in the chemical industry could result in wider acceptance of the methods in the industry, as well as the increased willingness of software vendors to develop their application interfaces

Publicity to the U.S. chemical industry regarding the advanced level of chemometrics activities at several foreign competitor companies needs to be done to raise the awareness of our international position regarding this technology.

A government-based, ATP research and development program to develop hierarchical, component-based software is needed to enable sustained and more timely development of more user-friendly development and implementation tools.

SUMMARY

The products of this workshop, as summarized in the preceding sections, were the identification of key challenges and needs in the area of process measurement and control with application to industrial operations. The specific needs were grouped under the following core technology bundles:

- Nonlinear model predictive control

- Performance monitoring
- Estimation and inferential control
- Identification and adaptive control
- Molecular characterizations and separations
- Process sensors
- Microfabricated instrumentation
- Information and data handling

In addition, a number of research priorities were identified as effective investments to meet the previously described challenges. Although a large number of specific priorities were identified within each group, the following common issues arose in many of the groups:

- Improved modeling approaches for large-scale, complex, nonlinear systems
- Quantitative metrics to evaluate the success of a particular approach, as well as the benefit to industry
- Better quantitative connections between final product properties and measurable quantities

Finally, a number of action items were enumerated to facilitate the accomplishment of these research needs. Regardless of the specific technology bundle, a few common recommendations for action items have emerged:

- Find a way to create a completely new entity modeled after Germany's Fraunhoffer Institutes to facilitate the interface among industry, academia, and government. Another effective model, cited often, was the CAPE-OPEN initiative in Europe for standardization of simulation technology.
- Conduct workshops jointly with industry, academia, and government, exchanging information on measurement and control challenges and capabilities. Make better use of WEB pages to communicate such material.
- Establish effective industry/university consortia consisting of multiple industrial partners as well as *multiple* university partners. Leverage industry support through government initiatives such as the NSF IUCRC program.
- Work toward changing academic attitudes toward industrial measurement problems. Institute industrial co-ops in chemistry and chemical engineering.
- Encourage government funding for industrial sabbaticals for university professors. Encourage the academic sabbatical idea amongst industrialists.
- Encourage academic training in problem-solving teamwork approaches, as well as hands-on training for both engineers and chemists with measurement devices and controllers.
- Establish meaningful industrial benchmark problems for the evaluation of new measurement and control technology, including a metric for evaluation. Provide forums to review progress by academics.

It was clear from both the active participation of many chemical industry representatives at the Workshop, and the ensuing discussion, that all participants at the Workshop view process measurement and control as key enabling technologies to the economic and environmental viability of the chemical industry. Advances in the areas enumerated in the document are crucial challenges to achieving the chemical industry goals advanced in *Vision 2020*.

APPENDIX I: Workshop Attendees

Workshop Planning Group Members

Maria Burka	NSF
Frank Doyle	University of Delaware
Arlene Garrision	University of Tennessee
Bruce Johnson	DuPont Company
Hratch Semerjian	NIST
Dave Smith	DuPont Company
Bob Watters	NIST

Workshop Speakers/Discussants

Steve Brown	University of Delaware
Lloyd Burgess	University of Washington
Ray Chrisman	Dow
Purnendu Dasgupta	Texas Tech University
Vince Grassi	Air Products
Mike Henson	LSU
Evelio Hernandez	Shell Oil Company
Bruce Johnson	DuPont Company
Ferhan Kayihan	IETek
Charles Miller	DuPont Company
Mike Nikolaou	University of Houston
Tunde Ogunnaike	DuPont Company
Joe Qin	University of Texas
Mike Ramsey	Oak Ridge National Laboratory
Masoud Soroush	Drexel University
Bob Watters	NIST

Workshop Participants

Yaman Arkun	Georgia Institute of Technology
Tom Badgwell	Rice University
Chuck Bartholomew	NIST
Karl Booksh	Arizona State University
Phil Carlberg	Dow
Ali Cinar	Illinois Institute of Technology
Paul Gemperline	East Carolina University
Christos Georgakis	Lehigh University
Jay Grate	Pacific Northwest National Laboratories
Paul Gusciora	Chevron
Mel Koch	University of Washington
Del Lawson	3M
Sue Matz	Equistar
Leslie May	Dow
Charlie Moore	University of Tennessee
Ken Muske	Villanova University
Jose Olivaros	Los Alamos National Laboratories
Ahmet Palazoglu	UC Davis
Larry Ricker	University of Washington
Dan Rivera	Arizona State University
James Rodgers	Solutia
Greg Rosasco	NIST
Eva Sevick-Muraca	Purdue University
Robert Siegmund	Ciba Specialty Chemicals
Lois Weyer	Hercules
Steve Wright	Argonne National Laboratory
John Zhu	Honeywell

APPENDIX II: Workshop Program

FRIDAY, MARCH 6, 1998

(Main Meeting Room – Tennessee Williams)
1:00 p.m. Welcome
Frank Doyle, Delaware
Dave Smith, DuPont
Maria Burka, Chemical and Thermal Systems, NSF
Bob Watters, NIST

1:15 p.m. Molecular Characterization and Separations, *Bruce Johnson*, DuPont
1:55 p.m. Discussant Comments, *Bob Watters*, NIST
2:05 p.m. Open Discussion

2:15 p.m. Nonlinear MPC, *Mike Henson*, LSU
2:55 p.m. Discussant Comments, *Evelio Hernandez*, Shell
3:05 p.m. Open Discussion

3:15 p.m. ***Coffee Break***

3:45 p.m. Sensors, *Lloyd Burgess*, U. Washington
4:25 p.m. Discussant Comments, *Ray Chrisman*, Dow
4:35 p.m. Open Discussion

4:45 p.m. Controller Performance Monitoring, *Joe Qin*, Texas
5:25 p.m. Discussant Comments, *Ferhan Kayihan*, IETek
5:35 p.m. Open Discussion

7:30 p.m. ***Organized dinner with discussion***
Group I – Alex Patouts
Group II – Jaeger's House of Seafood
Group III – The Palace Café
Group IV – Café Sbisa

SATURDAY, MARCH 7, 1998

7:30 a.m. ***Continental Breakfast***

8:00 a.m. Breakout Sessions
I. Molecular Characterization (Leader: *Bob Watters*) **Main Meeting Room (Tennessee Williams)**
II. Nonlinear MPC (Leader: *Evelio Hernandez*) **Rex Room**
III. Sensors (Leader: *Ray Chrisman*) **Crescent Room (4th floor)**
IV. Performance Monitoring (Leader: *Ferhan Kayihan*) **Edgewood Room (4th floor)**

10:30 a.m. Reports on Breakout Sessions

12:00 noon ***Catered lunch (hotel)***

1:15 p.m. Estimation and Inferential Control, *Masoud Soroush*, Drexel
1:55 p.m. Discussant Comments, *Tunde Ogunnaike*, DuPont
2:05 p.m. Open Discussion

2:15 p.m. Microfabricated Instrumentation Systems, *Mike Ramsey*, Oak-Ridge
2:55 p.m. Discussant Comments, *Purnendu Dasgupta*, Texas Tech
3:05 p.m. Open Discussion

3:15 p.m. ***Coffee Break***

3:45 p.m. Identification and Adaptive Control, *Mike Nikolaou*, Houston
4:25 p.m. Discussant Comments, *Vince Grassi*, Air Products
4:35 p.m. Open Discussion

4:45 p.m. Information and Data Handling, *Steve Brown*, Delaware
5:25 p.m. Discussant Comments, *Charles Miller*, DuPont
5:35 p.m. Open Discussion

7:30 p.m. ***Organized dinner with discussion (off-hotel restaurants)***

SUNDAY, MARCH 8, 1998

7:30 a.m. ***Continental Breakfast***

8:00 a.m. Breakout Sessions
V. Inferential Control (Leader: *Tunde Ogunnaike*) **Main Meeting Room (Tennessee Williams)**
VI. Microfabricated Instrumentation Systems (Leader: *Sandy Dasgupta*) **Rex Room**
VII. Adaptive Control/Identification (Leader: *Vince Grassi*) **Crescent Room (4th floor)**
VIII. Data Handling (Leader: *Charles Miller*) **Edgewood Room (4th floor)**

10:00 a.m. Reports on Breakout Sessions

11:30 a.m. Closing Comments

12:00 noon ***Catered lunch (hotel)***

1:15 p.m. Meeting of Workshop Organizers and Session Discussants to frame preliminary workshop report.

APPENDIX III: Breakout Groups

Molecular Separations & Characterizations (Sat. am) Estimation and Inferential Control (Sun. am)
Bruce Johnson (Speaker)
Masoud Soroush (Speaker)
Bob Watters (Discussant)
Tunde Ogunnaike (Discussant)
Leslie May
Karl Booksh
Charlie Moore
Sue Matz
Jose Olivaros
Yaman Arkun
Christos Georgakis
Larry Ricker

Nonlinear MPC (Sat. am) Microfabricated Instrument Systems (Sun. am)
Mike Henson (Speaker)
Mike Ramsey (Speaker)
Evelio Hernandez (Discussant)
Sandy Dasgupta (Discussant)
Phil Carlberg
Ahmet Palazoglu
Steve Wright
Frank Doyle
Mel Koch
Bob Siegmund
James Rodgers
Chuck Bartholomew

Sensors (Sat. am) Identification & Adaptive Control (Sun. am)
Lloyd Burgess (Speaker)
Mike Nikolaou (Speaker)
Ray Chrisman (Discussant)
Vince Grassi (Discussant)
Jay Grate
Del Lawson
Eva Sevick-Muraca
Paul Gusciora
Ken Muske
Dan Rivera
Dave Smith

Performance Monitoring (Sat. am) Information and Data Handling (Sun. am)
Joe Qin (Speaker)
Steve Brown (Speaker)
Ferhan Kayihan (Discussant)
Charles Miller (Discussant)
Ali Cinar
Tom Badgwell
John Zhu
Maria Burka
Arlene Garrison
Paul Gemperline
Lois Weyer
Greg Rosasco

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