Process Modeling and Control: A Vision of the Future

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1.0 Introduction

Much of the progress of process modeling and control over the past 20 years can be attributed to the continuing advances in digital computing. The development of the microcomputer and the 100-fold increase in computer speed each decade has led to significant reductions in hardware cost for computers of all types, including those in process control applications. Computers are pervasive, as is evident from the estimated 10 billion microprocessors and microcomputers in the world. The emergence of standard software packages and architecture has also facilitated applications in process control.

Forecasted future improvements in process modeling and control are a major component in the recently completed report, "Technology Vision 2020: Report of the U.S. Chemical Industry" [1]. This report was sponsored by five major societies and associations (AIChE, ACS, CCR, CMA, and SOCMA) referred to as the Chemical Enterprise Consortium (CEC), and involved more than 200 business and technical leaders from industry, academia and government. It presents a roadmap for the next 25 years for the chemical and allied industries, but it is an evergreen document to be consulted and updated as the chemical enterprise moves into the 21st century. Vision 2020 also provides a means for dialog and cooperation among all stakeholders in the chemical enterprise. The collaboration among CEC societies has spawned many additional workshops, generating more detailed R&D roadmaps on specific areas of chemical technology.

The modeling and control issues identified in Vision 2020 include changes in the way plants operate, computer hardware improvements, the merging of models for design, operations, and control, and developments in advanced control. It is estimated that by 2020 60% of industrial chemical production capacity will be characterized by high-yield or high-quality processes that generate near-zero waste or discharge. More recycled raw materials will be used as feedstocks. This will be driven mainly by modifying many processes; for example, organic solvents will be phased out in favor of using no solvents or aqueous solvents. In addition, there will be growing applications (about 10% of new processes) that use non-traditional chemistry (e.g., plasma, microwave, photochemical, biochemical, supercritical, and cryogenic).

2.0 Hardware and Software Changes

Further movement towards the Computer-Integrated Manufacturing (CIM) paradigm is expected. CIM is defined as a unified network of computer hardware and software systems that combines the business and process functions (such as administration, economic analysis, scheduling, design, control, operations, etc.). Operations will be guided by complete information, i.e., integration of sales, marketing, manufacturing, supply, and R&D data where data and information flow in a seamless fashion along the whole supply chain. CIM provides general access to a common data base and produces reports for managers, engineers, and operations so that optimum decisions can be made and executed in a timely and efficient manner. CIM is recognized as an important tool for improving the competitiveness of the U.S. process industries, but CIM is not yet implemented in a significant number of plants. Cooperation among computer vendors is required to develop a satisfactory computer/communication/software system.

We are now beginning to see a new stage in the evolution of plant information and control architectures because of the CIM paradigm. The last 20 years of progress in computer control has been spurred by acceptance across a wide spectrum of vendors of the distributed control hub system for process control, which was pioneered during the 1970s by Honeywell. A distributed control system (DCS) employs a hierarchy of computers, with a single microcomputer controlling 8 to 16 individual control loops. More detailed calculations are performed using workstations, which receive information from the lower-level devices. Set points, often determined by real-time optimization, are sent from the higher level to the lower level.

With the focus now on enterprise integration, automation vendors are now implementing Windows NT as the new solution for process control, utilizing personal computers in a client-server architecture rather than the hub-centric approach used for the past 20 years. This promotes an open application environment (open control systems) and makes accessible the wide variety of pc object-oriented software tools that are now available.

The demand for smart field devices is rising rapidly. In the CIM paradigm, one ought to be able to query a remote instrument and determine if the instrument is functioning properly. Of course digital-based rather than analog instruments have the key advantage that signals can be transmitted digitally (even by wireless) without the normal degradation experienced with analog instruments. In addition, smart instruments have the ability to perform self-calibration and fault detection/diagnosis. Smart valves include PID control resident in the instrument, which can permit the central computers to do more advanced process control and information management. It is projected that installations of smart instruments can reduce instrumentation costs by up to 30% over conventional approaches. There has been much recent activity in defining standards for the digital, multidrop (connection) communications protocol between sensors, actuators, and controllers. In the U.S. the concept is called fieldbus control, and vendors and users have been working together to develop and test interoperability standards via several commercial implementations.

When data become readily available at a central point, it will be easier to apply advanced advisory systems (e.g., expert systems) to monitor the plant for performance as well as detect and diagnose faults. Recent efforts have built on the traditional single variable SPC approach and extended it to multivariable problems (many process variables and sensors) using multivariate statistics and such tools as principal component analysis. These techniques can be used for sensor validation to determine if a given sensor has failed or exhibits bias, drift, or lack of precision.

In the area of process modeling industrial groups are beginning to examine whether it is possible to achieve a seamless transition between models used for design and simulation and models used for control. The CAPE-OPEN industrial consortium in Europe and other groups in the U.S. are working towards an open architecture for commercial simulators to achieve "plug and play" using company-specific software such as physical property packages. The extension of these steady-state flowsheet simulators to handle dynamic cases is now becoming an active area (e.g., linking Aspenplus to Speedup). The goal is to have models for real-time control that run at 50 to 500 times real-time, but this will require increased computational efficiency and perhaps application of parallel computing.

3.0 Developments in Model-Based Control

A new generation of model-based control theory has emerged that is tailored to the successful operation of modern plants, addressing the "difficult" process characteristics encountered in chemical plants shown in Table 1.

Table 1

Process Characteristics That Must Be
Treated by Advanced Control

- Time Delays
- Nonminimum Phase
- Disturbances
- Unmeasured Variables
- Noise
- Time-Varying Parameters
- Nonlinearities
- Constraints
- Multivariable Interactions

These advanced algorithms include model predictive control, robust control, and adaptive control [2, 3], where a mathematical model is explicit in developing a control strategy.

The success of Model Predictive Control (MPC) in solving large multivariable industrial control problems is impressive. Model predictive control of units with as many as 10 inputs and 10 outputs is already established in industrial practice. Computing power is not causing a critical bottleneck in process control, but larger MPC implementations and faster sample rates will probably accompany faster computing. Improved algorithms could easily have more impact than the improved hardware for the next several years. MPC will appear at the lowest level in the DCS, which will reduce the number of PID loops implemented.

Adaptive control implies that the controller parameters should be adapted in real-time to yield optimal performance at all times; this is often done by comparing model predictions with on-line plant data and updating the process model parameters. The use of nonlinear models and controllers is underway in some applications. Some of the new versions of MPC are incorporating model adaptation, but so far adaptive control has not had much impact. This is due to problems in keeping such loops operational, largely because of the sensitivity of multivariable adaptive controllers to model mismatch.

In MPC control actions are obtained from on-line optimization (usually by solving a quadratic program or QP), which handles process variable constraints. MPC also unifies treatment of load and set-point changes via the use of disturbance models and the Kalman filter. MPC can be extended to handle nonlinear models, as shown in Figure 1.

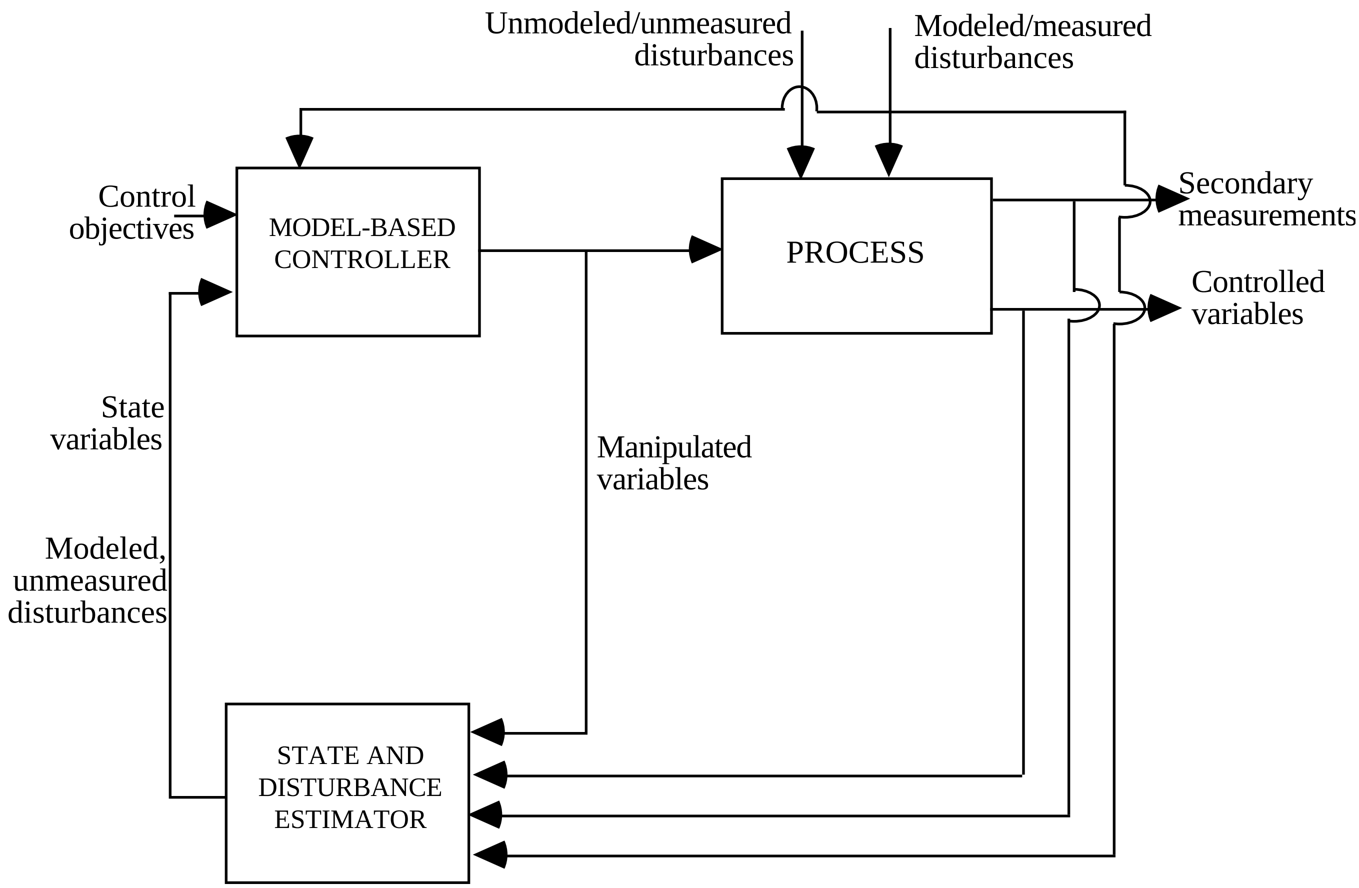

Figure 1. Generalized Block Diagram for Model Predictive Control

Recent announcements by software vendors indicate that the combination of process simulation, optimization, and control into one software package will be a near-term reality, at least if some corporate mergers and acquisitions are any indication, Aspentech's acquisition of Dynamic Matrix Control Corporation, Setpoint, Inc., and Neuralware will provide the ability to offer integrated technology with a set of consistent models across R&D, engineering, and production stages, with increased emphasis on rigorous dynamic models and the best control solutions. Similarly, Shell Oil Company and Simulation Sciences are developing a new modeling software system called rigorous on-line modeling and equation-based optimization

(ROMEO). Simulation Sciences was recently acquired by Siebe, who also owns Foxboro. Software users will be able to optimize plant-wide operations using real-time data and current economic objectives. The equation-based approach is expected to be faster than the sequential-modular (unit operation) methodology. The software can determine the location and cause of operating problems and provides a unified framework for data reconciliation and parameter estimation in real-time.

There are still many questions to be answered regarding the connection between modeling and control. For example:

(1) What explicit modeling information is required to achieve a particular level of control performance?

(2) Even in the case of perfect models, what are the fundamental limitations on control performance?

(3) What are the tradeoffs between modeling accuracy, control performance, and stability?

Developing the answers to these questions is the subject of current research.

Process Control in 2020

In the factory of the future, the industrial environment where process control is carried out will be different than it is today. In fact, some forward-thinking companies believe that the operator in the factory of the future may need to be an engineer as done in Europe. Because of greater integration of the plant equipment, tighter quality specification, and more emphasis on maximum profitability while maintaining safe operating conditions, the importance of process control will increase. Very sophisticated computer-based tools will be at the disposal of plant personnel. Controllers will be self-tuning, operating conditions will be optimized frequently, fault detection algorithms will deal with abnormal events, total plant control will be implemented using a hierarchical (distributed) multivariable strategy, and expert systems will help the plant engineer make intelligent decisions (those he or she can be trusted to make).

Plant data will be analyzed continuously, reconciled using material and energy balances and nonlinear programming, and unmeasured variables will be reconstructed using parameter estimation techniques. Digital instrumentation will be more reliable, will be self-calibrating, and composition measurements which were heretofore not available will be measured on-line. There are many industrial plants that have already incorporated several of these ideas, but no plant has reached the highest level of sophistication over the total spectrum of control activities. Figure 2 illustrates a possible hierarchical CIM structure that could be used in merging business optimization with plant and process operations and control. Each layer will have different models and time scales and includes checking the model against data obtained by the computer systems.

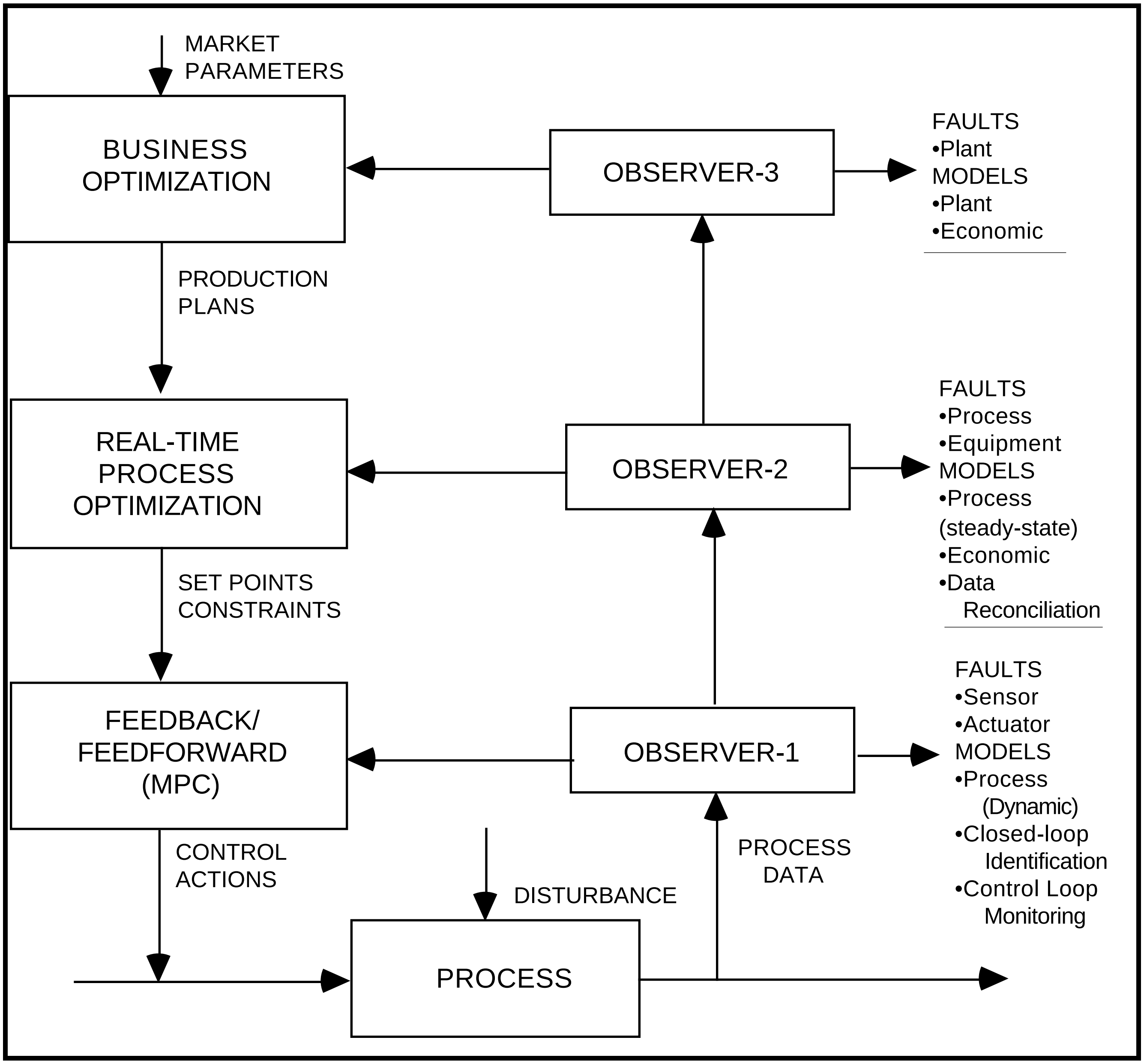

Figure 2. Computer-Integrated Manufacturing: Combining Business and Process Operation Using Computer Control (Adapted from Stephanopoulos [4])

4.0 Technology Roadmaps in Process Instrumentation, Control, and Operations

Since the issuing of the Vision 2020 report in 1996, organizations including CCR, ACS, and AIChE in conjunction with sponsorship by government agencies such as NSF, NIST, DOE, and EPA have been holding workshops to develop technology roadmaps. Several workshops pertinent to this presentation have been held during 1997 and 1998, and other Vision 2020 workshops have been held on subjects such as separations, catalyst synthesis, polymer research in green chemistry and engineering, and computational fluid dynamics. See http://www.chem.purdue.edu/v2020/ for the CCR (Council for Chemical Research) Vision 2020 web site.

Chemical Instrumentation

Chemical analysis is a critically important enabling technology essential to every phase of chemical science, product and process development, and manufacturing control. 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 microscopes, scanning spectral analysis, and the integration of computers with instrumentation. These methods have been extended to the detection and spectral characterization of molecular structure at the atomic level.

A workshop was held in March, 1997, to assess future directions for R&D in chemical instrumentation. Research needs identified included:

- transfer of analytical laboratory capabilities into plants, incorporating ease of maintenance and support, utilizing new technology and molecular scale devices

- improved real-time characterization of polymers (molecular weight distribution, branching)

- improved structure/property/processing modeling capability, especially macromolecular products such as biomolecules and biopolymers

- physical/chemical characterization of solids and slurries

- on-line characterization of biotechnological processes

- new approaches for sampling and system interlinks to control and information systems

- self-calibrating and self-diagnostic (smart) sensors

- identification of processes needing microfabricated instruments and development of corresponding models/control systems

- integration of data from multiple sensors for environmental compliance, product development, and process control, including soft sensors.

- advanced measurement techniques to support combinatorial chemistry in catalysis and drug discovery

For more details see the URL www.nist.gov/cstl/hndocs/ExternalTechnologyBundles.html.

Process Measurement and Control

In recognition of the needs and challenges in the areas of process measurement and control, a workshop entitled "Process Measurement and Control: Industry Needs" was convened in New Orleans, March 6-8, 1998. Approximately 50 participants attended from academia, industry and government laboratories. Publications from the workshop will appear in a special issue of *Computers and Chemical Engineering* in the future. The goals of the workshop were:

(1) To survey the current state-of-the-art in academic research and industrial practice in the areas of measurement and control, particularly as they apply to the chemical and processing industries. The extent of integration of measurements with control is a particular focus of the survey;

(2) To identify major impediments to further progress in the field and the adoption of these methods by industry; and

(3) To determine highly promising new directions for methodological developments and application areas.

The workshop emphasized future development and application in eight areas:

- Molecular Characterization and Separations
- Nonlinear Model Predictive Control
- Information and Data Handling
- Controller Performance Monitoring
- Sensors
- Estimation and Inferential Control
- Microfabricated Instrumentation Systems
- Adaptive Control and Identification

See http://fourier.che.udel.edu/~doyle/V2020/Index.html for further information on workshop findings.

As an example of a specific roadmap the first topic (nonlinear model predictive control or NMPC) has been mainly of academic interest so far, with a few industrial applications involving neural nets. What is needed is an analysis tool to determine the appropriate technology (NMPC vs. MPC) based on the process description, performance objective, and operating region. There is also a desire to represent complex physical systems so that they are more amenable to optimization-based (and model-based) control methods. The improved modeling paradigms should address model reduction techniques, low-order physical modeling approaches, maintenance of complex models, and how common model attributes contribute pathological features to the corresponding optimization problem. Hybrid modeling, which combines fundamental and empirical models, and methodologies for development of nonlinear models (e.g., input sequence design, model structure selection, parameter adaptation) deserve attention. More details are contained in the URL for this workshop.

Process Operations

Another workshop in a related area, Systems Technologies for Process Operations, was convened after the FOCAPO meeting in Snowbird, Utah in July 10-11, 1998. The objective for the workshop was to review and to distill the technology needs and research ideas generated from the 150 participants at the FOCAPO conference and, as necessary, to supplement these with ideas from the workshop panel. A list of needs and challenges for this field, as well as new capabilities, improvements, and enhancements of existing technology that will be required to address the long range needs in the operations domain. Furthermore, broad estimates of the time and funding required to arrive at these new capabilities and enhancements as well as the priorities among them were made. The workshop report will lead to a technology roadmap, which will be developed by a subgroup of this panel [5].

References

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