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Modeling, simulation, optimization and control of chemical process Case study: oil and gas up streams

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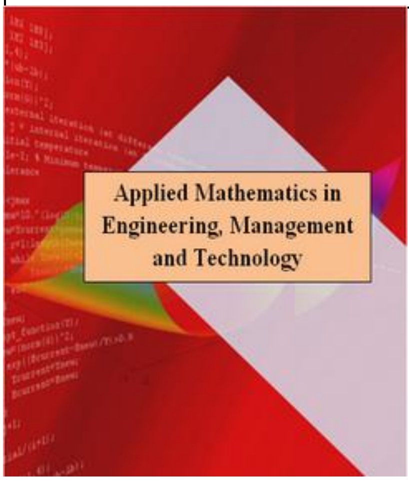


Abstract:

This paper investigates a common framework in the field of Modeling, simulation ,optimization and control of chemical process with the emphasis on the oil industry. Oil and its deviations are very important substances and have an inevitable impact on the mankind's role. In this regard, the prediction of its properties and operations could be very important and is necessary to draw an optimal process so as to minimize the waste and decreasing the costs of refinery. At first, some basic definitions are presented and after that a common framework is presented so as to reach an optimal process optimization.

1. Introduction

Oil is a very important substance and has an inevitable impact on the mankind's role. In this regard, the prediction of its properties and operations could be very important and is necessary to draw an optimal process so as to minimize the waste and decreasing the costs of refinery. At first, some basic definitions are presented and after that a common framework is presented so as to reach an optimal process optimization.
Process optimization is a set of activities in order to optimize some specified set of parameters without violating some constraint. The most common goals are minimizing cost, maximizing throughput, and/or efficiency. This is one of the major quantitative tools in industrial decision making.
When optimizing a process in oil industry, it is aiming to to maximize one or more of the process specifications which are effective on refinery procedure could be lead the total costs of refinery to be decreased, while keeping all others within their constraints.
Fundamentally, there are three parameters that can be adjusted to affect optimal performance. They are:

- Equipment optimization

The first step is to verify that the existing equipment is being used to its fullest advantage by examining operating data to identify equipment bottlenecks.

- Operating procedures

Operating procedures may vary widely from person-to-person or from shift-to-shift. Automation of the plant can help significantly. But automation will be of no help if the operators take control and run the plant in manual.

- Control optimization

In a typical processing plant, such as a chemical plant or oil refinery, there are hundreds or even thousands of control loops. Each control loop is responsible for controlling one part of the process, such as maintaining a temperature, level, or flow.
If the control loop is not properly designed and tuned, the process runs below its optimum. The process will be more expensive to operate, and equipment will wear out prematurely. For each control loop to run optimally, identification of sensor, valve, and tuning problems is important. It has been well documented that over 35% of control loops typically have problems. The process of continuously monitoring and optimizing the entire plant is sometimes called performance supervision.
The highest level of optimization includes the optimization of the raw material supply chain and the optimization of the packaging and product distribution chain. The plant wide optimization must consider documentation, maintenance, scheduling, and quality management considerations. Plant wide optimization resolves the conflict of objectives between the unit operations and the envelope strategies required to optimize the entire plant. Within the unit operations level multivariable optimization cannot be achieved when individual

processing equipment is defective or when the control loops are not properly tuned. It is important that measurements be sampled fast enough, that controls loops be tuned for fast rates of recovery, and loop cycling be eliminated. When no mathematical model can describe a process, the process can only be optimized experimentally and empirical optimization is required .

Optimization Design

Constraints
Design constraints are physical limitations or restrictions that must be satisfied to produce an acceptable design [1].

- Operation conditions – safety, environmental
- Equipment constraints – e.g. pump rates
- Storage capacities
- Product quality and impurities

Optimization Situations
The following list describes common reasons for optimization in an industrial plant.

- Sales limited by production (e.g. reduce costs by minimizing downtime)
- Sales limited by market (e.g. be the “low cost producer”)
- Plants with high throughput
- High raw material or energy consumption
- Product quality better than specifications
- Loss of valuable or hazardous components through waste stream

Real-Time Optimization
The following describes the steps in order to optimize a chemical engineering process.

1. Identify process variables
2. Select objective function (e.g. profit $$$)
3. Develop process model and constraints
4. Simplify model to objective function (e.g linearization)
5. Compute the optimum
6. Perform sensitivity study

Industry Experience
Optimization can be applied to every aspect of a process. For example, at a refinery there are operators that work out in the units. Optimization can be applied to increase the operator/engineer communication by implementing "real-time" computer programs that allow the process engineers to see what is actually happening in the plant. This will help optimize process by allowing engineers to see what the conditions in the plant are in real time.

Pilot Plant Experience
Optimization of processes in a pilot plant will allow for more efficient scale-up to commercial size. In the ChE 460 course, four unit operations are optimized to produce soybean biodiesel. In order to optimize the reaction conversion, the project engineers vary catalyst concentration, agitation rate, and temperature. A design of experiment (DOE) is used to find the best set of input parameters.

2. Research main study

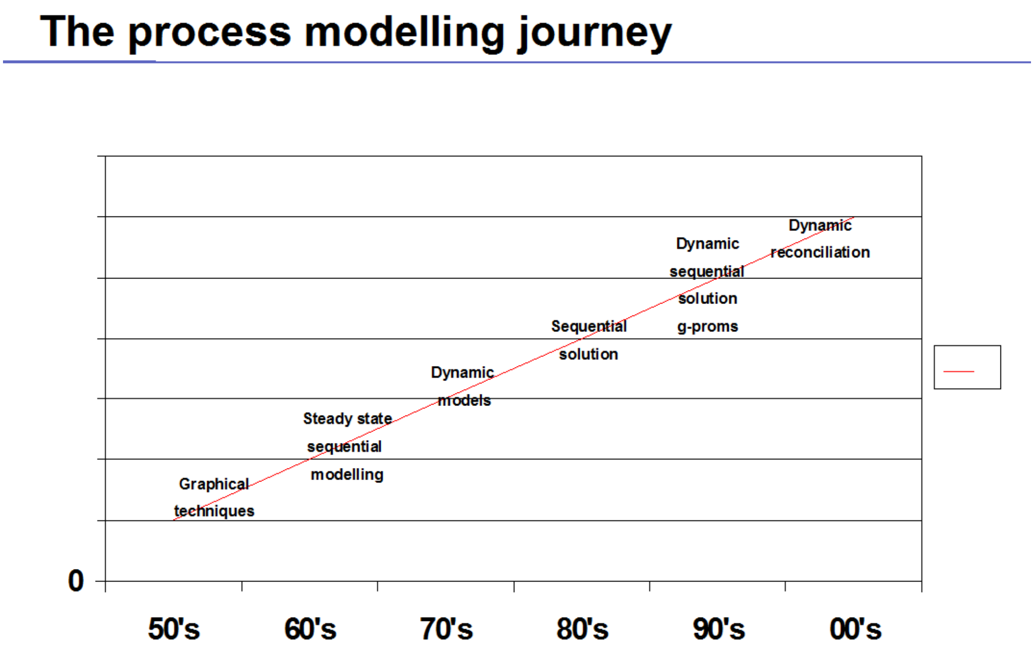
The main subject of this paper is to build a common experience during in the process industries and on everything about process control in real life industry. The main fields which are studied in this paper are in the following areas:

- Process Modeling
- Process Control
- Digital Communication
- Supply Chain Performance

All four are approaching a common point that demands smart control for tomorrow's processes.

2.1.Process modeling

The process industries involve some form of chemical or physical transformation. These transformation processes are often non-linear and poorly understood. Preparing a dynamic model is difficult. A typical example would be an agrochemical batch reactor with complex kinetics, including main and side reactions.



In the early sixties, Professor Roger Sergeant at Imperial College (1), researchers at ICI and others started to explore the potential for using computers to solve the basic unit operations of chemical engineering. Prior to that time, graphical techniques were used to design basic unit operations, such as distillation columns. Given that the model of a distillation column is a series of counter-current equations, it was ideally suited to the early digital computers.

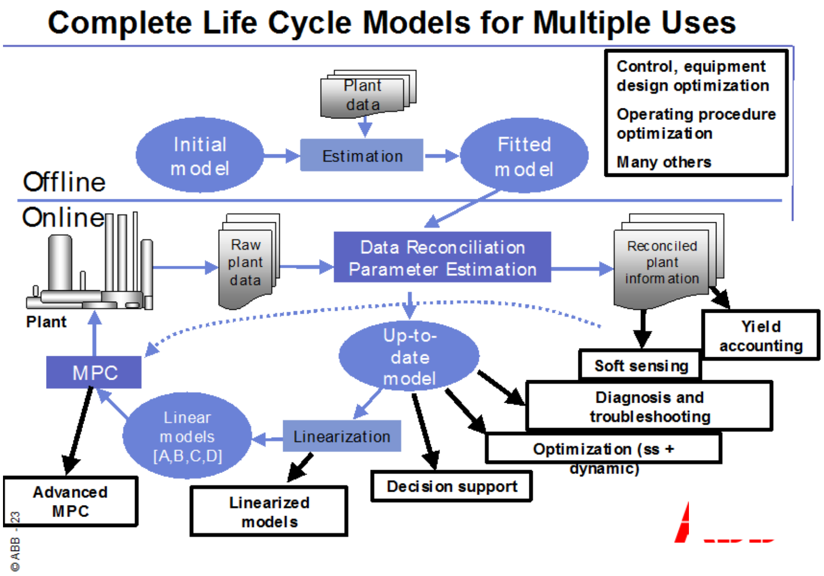
The goal in using computers was to significantly reduce the time and effort involved in modeling while improving the design accuracy. Models were totally steady state but nonetheless proved of great benefit. The techniques used involved flow sheeting languages that have since evolved into the solutions now offered by companies like Aspen and Hyprotech. These early models solved equations in a sequential manner that followed the process; that is, the model first solved the reactor equations and then used the outputs as the inputs to the distillation column. While this approach felt intuitively correct, the drawback was the relatively slow speed of solution.

In the late seventies, increasing computer power, plus research into basic mathematics and chemical engineering, encouraged researchers to consider dynamic process models. Again Imperial College was the leader and the result was the "Speed Up" product (2). This was eventually licensed by Aspen and is now a standard product that is available on the market. One of the drivers of these developments was to improve control of the chemical processes. As a generalization, chemical processes have considerable capacity in the form of tanks, reboilers, etc. This often means that the dynamics are relatively slow; hence, it was possible to tackle dynamic control problems using dynamic process models.

At around the same time, the concept of simultaneous equation-based solutions was developed. In this approach all the model equations are solved simultaneously. This brings real benefits in accuracy and speed. A key component of any process model is accurate physical properties data. Initially government laboratories developed these models. They have now been transferred to private owners, who develop and manage the core physical properties used by many of the process mathematical models.

Over the past 20 years, steady-state modeling moved from research to the norm in the industry, and the vast majority of engineers now use some form of steady-state modeling. This includes the Process Engineering Library (PEL) (Reference 3), which was originally developed by ICI and is available from ABB, and larger packages available from companies like Aspen.

In the nineties, the concept of combining equation-based solutions with dynamic models was advanced, again by Imperial College (Reference 4). The result was g-proms, the latest development in dynamic modeling and flow sheeting. ABB has an exclusive license for this technology in the automation area and has worked in partnership with PSE to develop their own version of g-proms applicable to the process industries. The key development is the dynamic data reconciliation module.

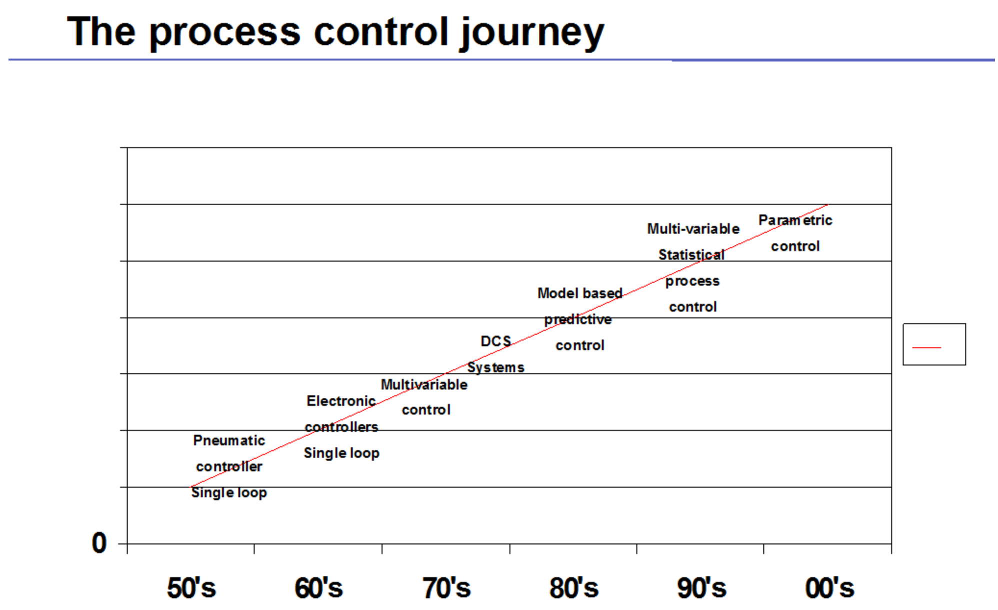


Dynamic reconciliation allows the user to ensure that all the heat and material balances of the process are reconciled at all times without having to wait for the process to attain steady state. This has numerous advantages to the user in the form of accuracy, removal of arguments on yields, and ability to monitor leak detection, instrument failures and heat exchanger efficiency, as well as provide “fit and forget” model-based predictive control.

Hence, the evolution of process modeling over forty years has made it possible to model dynamically almost any chemical process and to apply the latest advanced control techniques on a “fit and forget” basis. This means there is no longer a requirement for the time consuming step tests and recalibration of the previous multi-variable control models. Here is an example of how process modeling and process control are coming together to the benefit of the process industries.

2.2.Process control

Process control has also gone through a similar cycle over the last forty years. This is illustrated in the following diagram.



In this area the industrial applications have followed the research applications at universities.

In the fifties research focused on single loop controllers with the work of Bode and Nichols, who developed single loop control theory. The process industries followed, though initially they were inhibited by the limitations of pneumatic controllers. Advanced control was restricted to ratio or possibly feed forward control.

In the sixties universities such as UMIST began to develop the concept of multi-variable control with the work of Professor Alistair MacFarlane. In addition, the development of computer control demanded the development of the theory of sample data control. Only thirty years ago, control engineers such as the author had to argue the case for using computers to control process plants. Computers are now the norm.

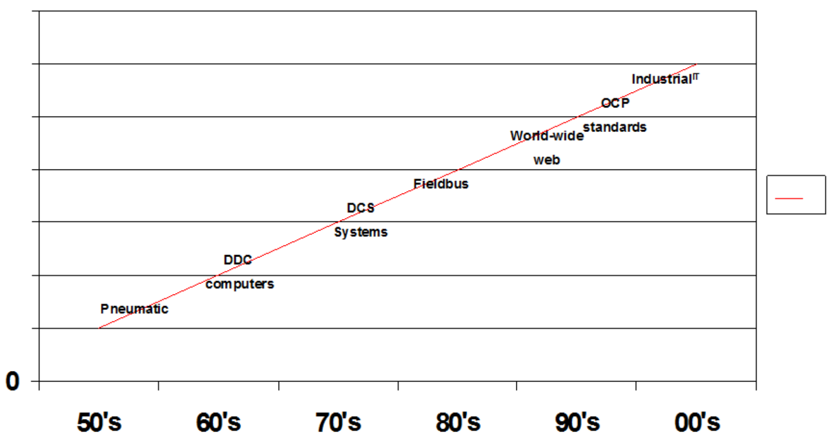
The key, however, to multi-variable control in the process industries was the development of model-based predictive control by Professor Manfred Morari and others in the late seventies. In this control a form of process model is inverted to provide feedback to the control variables. This concept was initially exploited industrially by Shell, and it was in the refining area that model-based predictive control really became established. This type of advanced control is increasingly the norm in the refining area, and it is also increasingly finding acceptance in other industries where advanced control is required. However, the problem with model-based predictive control is that it requires a dynamic model of the process. Normally engineers carry out numerous disturbance tests on the process to develop a dynamic model. While this approach proves quite effective until the process changes significantly, it is time consuming, and it is difficult to know exactly how good the model-based predictive control is compared with the best possible.

In the nineties the lessons learned from the non-process industries began to spread into the process industries. One only has to go round an electronics company or a car company to realize that their method of control is statistical process control. Terms like Six Sigma are growing in importance. This is a single variant form of control. The process industries are usually multi-variant. University research at Newcastle upon Tyne University and others has led to Multi-Variable Statistic Process Control (MVSPC). This applies the concept of statistical process control to the process industries. MVSPC is growing in importance, particularly in the batch processes, and will be very significant in the first ten years of the twentieth century.

In every case, the suppliers of process control equipment, such as ABB, have followed the lead provided by the universities, sometimes with a five-year or more gap between the research and the first commercial applications.

Forty years ago, many of the large process companies had large leading edge process control groups that were able to develop and prototype university research in industry before the equipment suppliers developed and offered them as standard products. Very few companies now retain this skill, and it is increasingly the obligation of supply companies such as ABB to be the direct translators of university research into industrial products. Increasingly such companies are becoming the first tier suppliers to the process industries.

The data communication and Industrial^{IT} control journey



On reflection, and not surprisingly, the key driver of this whole evolution has been the digital computer. Only forty years ago, the majority of process plants used pneumatic instrumentation. While in its own way pneumatic instrumentation was very clever and very simple, it was clearly very difficult to transfer data from these instruments to any form of central location. In fact the best that could be done was to have the operators manually record information that was manually analyzed by others. Rotating pneumatic scanning valves that converted pneumatic signals into digital signals were developed but these were restricted to a very few applications.

In the late sixties, the first direct use of computers to control process plants was achieved by ICI in the UK and Monsanto in the US. Unfortunately all the instruments and all the valves were pneumatic, hence numerous analogue-to-digital and digital-to-analogue converters had to be installed to make this approach possible. Nonetheless, the principle was established. Computer controls rapidly took off through the seventies and were installed in many large plants, primarily to allow innovations such as advanced control and optimization. For anybody who was working in that era, a real challenge was the need to communicate with numerous different standards of interfaces for pneumatics, electronics and other people's instruments.

This challenge led to an industry demand for a concept that eventually became known as Fieldbus. With Fieldbus, anybody's instruments can communicate with anybody's computers over a single standard interface. The author first heard of Fieldbus in the late seventies, and it is only now becoming the standard demanded by the industry. A gap of almost 30 years! The evolution of Fieldbus has been long and torturous, and it may well be suspected that it was not in everybody's interests to make it succeed.

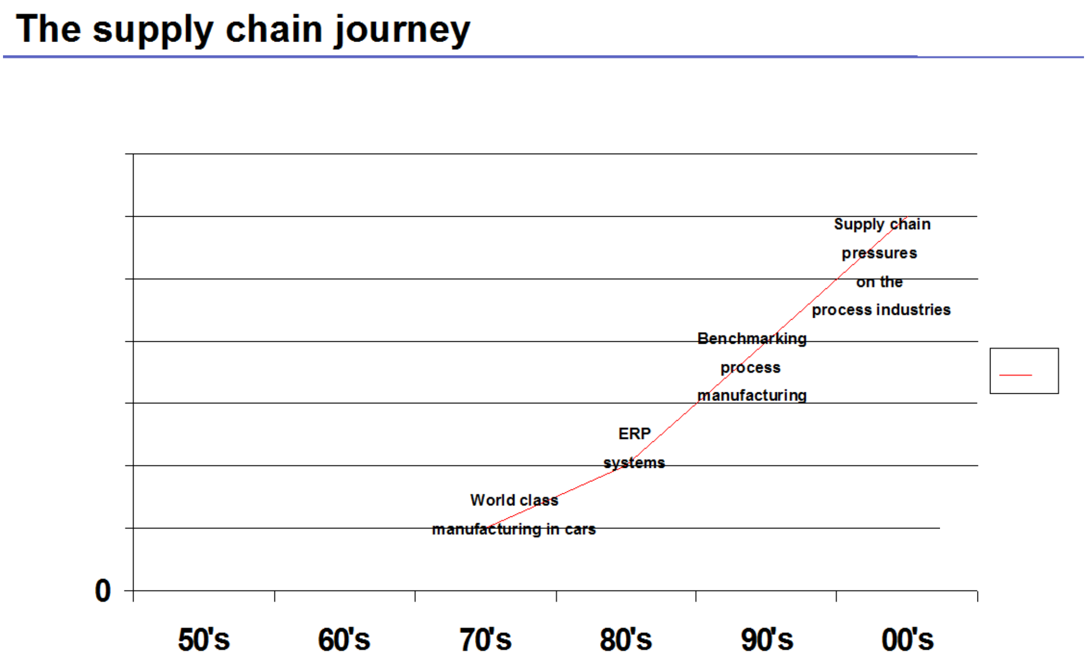
In the early nineties, the concept of the Internet and the worldwide web arose. This came from a totally different direction, and was developed for the totally different need of transferring huge amounts of data across the world using existing spare computer capacity. It involved nothing like the standardization effort of Fieldbus nor the numerous committees that made it possible. Nonetheless, the Internet rapidly gained acceptance as a worldwide standard because of its ease of use, availability and effective low cost. As a consequence, suppliers are now exploring the use of the web for communication between instruments and computers, etc., and it may eventually replace some components of Fieldbus.

In the nineties, ABB took a fundamental review of the whole question of information flow, both between plants and business systems and between components across plants. The result was the concept of Industrial^{IT} (3) .

To put the significance of Industrial^{IT} into context, it is probably appropriate to remind people that there was a time before Windows Office when letters were typed on typewriters and duplicates required carbon paper. That situation existed probably no more than thirty years ago. Within that time typewriters have disappeared, carbon paper is a museum piece, and Microsoft Office has become the standard for all offices in the world. ABB believes that Industrial^{IT} will become the standard for communication in the industrial world. The key and unique feature of Industrial^{IT} is the recognition that every object in the plant has information associated with it. ABB calls this information "aspects." Consider a typical control valve, which is an **object**, as illustrated in the following diagram.

2.3.Impact of supply chain

This is a much shorter but equally significant journey as illustrated below.



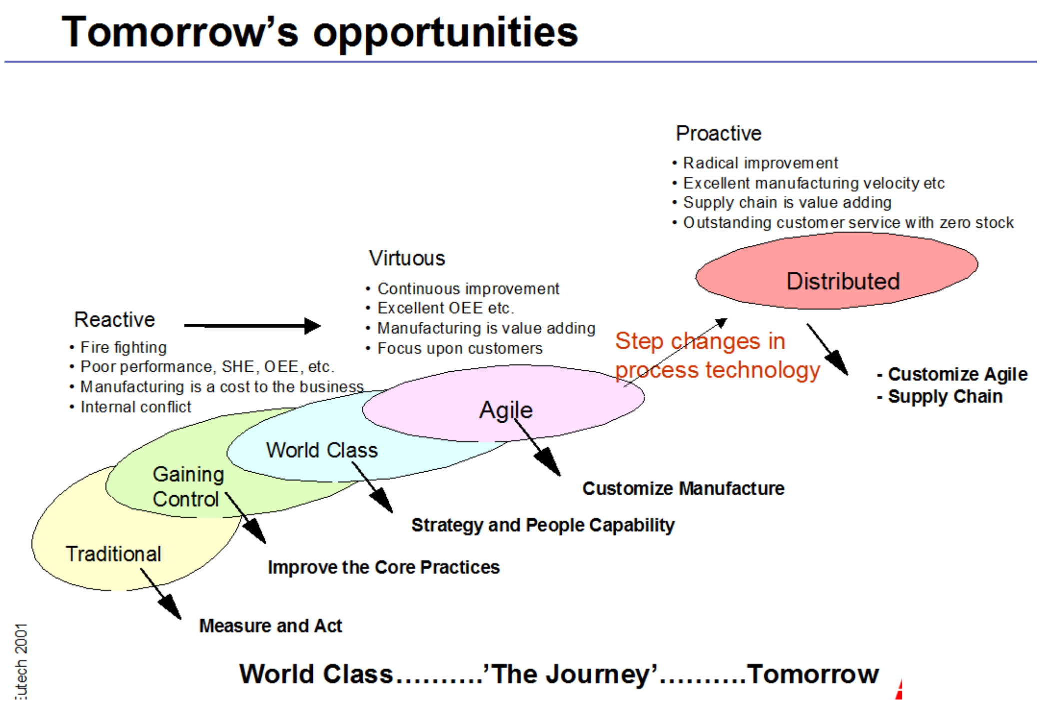
The process industries operate within a supply chain between raw materials supply (such as oil) and final customers (such as supermarkets). Strange as it may seem, this has not always been the case. In the sixties market demand exceeded supply in most products; hence, the only requirement was to ensure that you could produce the product. If the product was available, it sold; and how it was sold and the economics of sale were not really important.

Supply chain pressures did not really affect the process industries until the late eighties. The impact was felt earlier in industries such as cars and electronics. This led in the seventies to the concept of world class manufacturing of cars, which was first exploited in Japan and had significant impact on the western world in the late seventies. This concept led to a whole new manufacturing paradigm. Phrases such as lean manufacture and total productive management developed into a new industrial language.

In the early nineties, it began to be recognized that the concepts of world-class manufacturing applied to the process industries. The author would claim to be one of the people who brought this thinking into the industry. His book on benchmarking in process manufacturing (Reference 5) lays out some of the thinking behind world class manufacturing.

A key requirement of world class manufacturing is the recognition that you must benchmark against world class, and that the performance metrics refer to manufacturing performance, not process engineering performance. The table below lists some of these world class manufacturing metrics for Refining and Petrochemicals. Similar figures apply to batch processes.
Supply chain costs as a percent of sales is defined as follows: all the costs associated with the supply chain, excluding manufacturing, divided by the sales revenue. The costs include sales, marketing, the information management systems, the head office costs, the cost of warehouse, the cost of distribution, etc. You will see from the above table that a typical figure in the process industries is about 14% but we have experienced costs as high as 25%. World class is about 5-6%. Companies like Dell, Amazon and others in the leading edge markets set world class. Note that the difference between 5% and 14% is 9% of sales, which is an enormous figure that immediately impacts a company's bottom line. This is the fundamental reason why improving supply chain performance is a high priority task in many companies, and why it has accelerated rapidly up the agenda from a start in the nineties to become the hot topic in the first decade of the twentieth century.

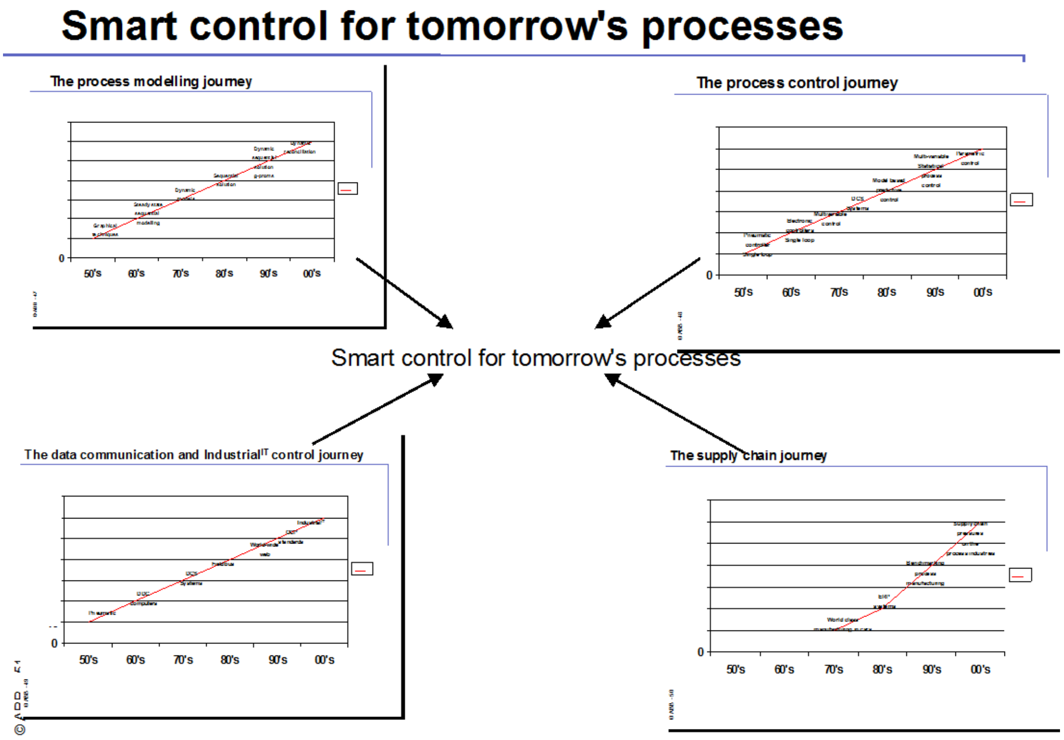
To deliver world-class manufacturing that delivers world leading supply chain performance will, in many cases, require radically different processes.



For example, world-class supply chain performance demands that you make to order with minimum raw material and finished goods stock. Unfortunately, many process plants were built twenty or thirty years ago when the philosophy was to run them steadily at a fixed rate, or to manufacture a large minimum batch size. The consequence of this is that you absorb swings in the market by using inventory. This approach is totally opposite to the requirements of a world-class supply chain. Incidentally, one of the reasons plants were built this way was a lack of understanding and process modeling adequate for the wide range of operations. Moving to a world-class supply chain demands processes that are capable of manufacturing "**to a unit of one**," as described by Manufacturing Foresight (Reference 6). This basically says that, if the customer orders one drum of chemicals, you make one drum of chemicals. If there are no orders, you do not manufacture. You need agile process manufacturing: plants that can be run at any rate automatically and provide perfect product. This concept is a natural introduction to the main topic of this paper.

Smart control for tomorrow's processes

All four of the trends identified are now approaching a common point where the market will demand smart control for the processes of tomorrow.



The prime driver is the market as represented by the supply chain. The final customers will always require just-in-time delivery, in full, of products with zero defects. This trend has been recognized in the UK Foresight exercise that recently led to a report called *Manufacturing 2020:We can make it!* (Reference 6). The report highlighted five significant themes for the future, which are summarized in the figure below.
Manufacture to a unit of one is the key flexibility driver. One interpretation of this driver is that the chemical plant has to be designed to produce a batch size equal to the smallest order size, even if the order size is one drum of chemicals. This demands manufacturing processes with the following characteristics:

- Design for minimum inherent volume and capacity
- Build quality into the whole process from beginning to end, such that Six Sigma performance is achievable.
- Smart sensors
- Totally accurate mathematical models
- Application of multi-variable statistical process control to monitor the operational process
- Direct link between the real-time plant and the business systems

Given what has been said earlier, the ability to provide a totally accurate dynamic model is possible with developments such as g-proms.

These requirements demand a wider spectrum of manufacturing processes, from ever-larger continuous plants at the source of feedstock, through to distributed, intensified and small plants that work on a made-to-order basis at the point of use. Throughout the spectrum the requirements will be for "smart operations" where the controls and the knowledge are used to match the process output and the quality to an ever more variable demand. Concepts like intensification at the University of Newcastle, flexible batch plants at the University of Imperial College and pipeless plants, as built by ICI and Mitsubishi, provide further options for tomorrow's processes. Hence, it is possible now to design a process for chemical manufacture that is agile. Note that the closer you are to the final consumer, the greater the need for agility. The converse is that the farther away you are from the consumer (in companies such as oil supply and raw materials processing), the less the need for agility and the more the processes (such as cat crackers and olefin plants) will remain unchanged. However, an interesting development is occurring in the form of gas-to-liquids technologies which would allow the hydrocarbon liquids to be made from gas, potentially at the point of use. This development could significantly change the nature of the supply chain.

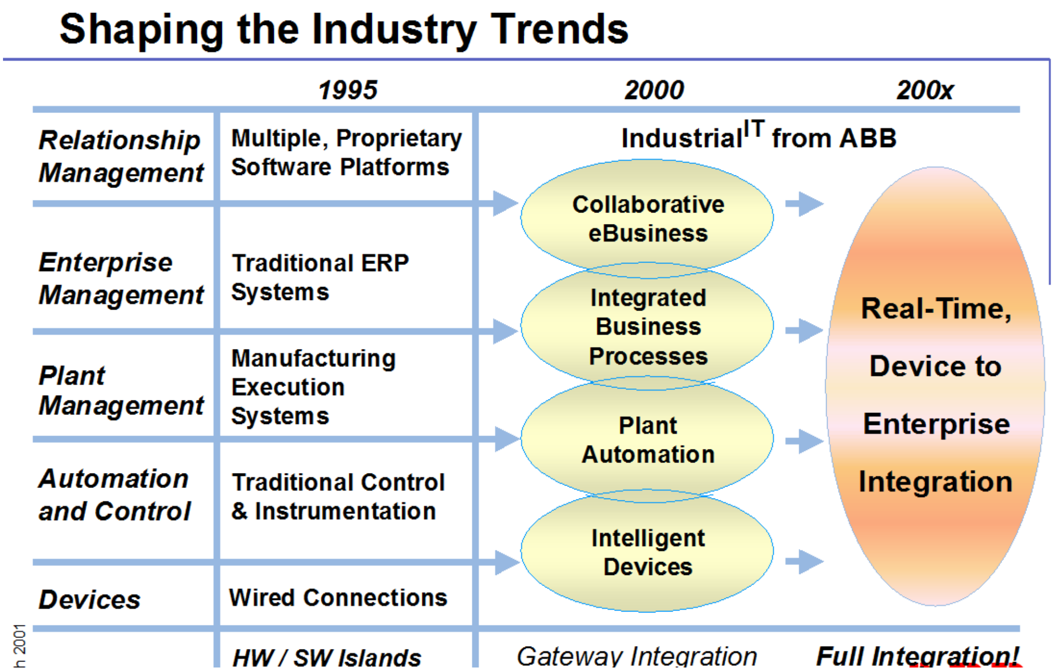
The rate of adaptation is presently inhibited by a belief that the process industries of the future will look like the process industries of the past. This is difficult to accept given the pressures that are coming from the supply chain. Driving down supply chain costs as a percentage of sales from 15% to 5-7% is just too large an incentive.

The pressure for tomorrow's processes to be agile means that they have to be designed to exploit the full potential of process control. That includes control of:

- The actual chemical processes
- The energy sources, such as electricity
- Safety, health and environment
- Maintenance management
- Supply chain operations

All the control will be in the context of multi-variable statistical process control, as the products will go straight to the customers without any laboratory testing or final product storage.

These "smart operations" will have the ability to make to order. This leads to the concept that the orders will arrive directly at the plant. The plant will purchase the raw materials as required, produce the products and ship them to the final customers. This basically says that the plant is managing the supply chain. Hence, there will no longer be a need for the vast centralized supply chain software being developed by many well-known companies. Instead, supply chain management will become distributed, managed by each plant. This trend is recognized by ABB and described as Real-Time Enterprise Integration.



This trend has major consequences for the costs of the supply chain in that it is no longer necessary to have large IT departments, HR departments, Accounts departments, etc., at some central location, incurring overhead. The whole supply chain will become green.

The supply chain is a dynamic system where the capacities are warehouses, distribution, order processing times, etc. It is possible to develop a dynamic model of the supply chain. In other words, control over the supply chain is a process control problem. Hence, one anticipates that tomorrow's smart control will apply all the techniques of single loop, multi-variable model-based predictive and multi-variable statistical process control to the concept of the supply chain.

One consequence will be to raise the benchmarks of world-class process plants closer to those of the leading software companies of today. Suggested targets are given below. (Reference 7)

Benchmarks for a flexible Chemical manufacturing

	Poor	Good	World class Today	World class Tomorrow
m hrs / Reportable injuries	0.01	0.1	>1	>10
Environmental incidents				0
OTIF %	40%	99.9%	>99%	>99.9 %
Customer Complaints (% of orders)	6%	0.01%	<0.1%	<0.0004%
Production rate	60%	99%	>90%	>99%
Quality rate	45%	99%	>99%	100%
Availability %	70%	96%	>95%	100%
OEE	20%	94%	>85%	>99%
Process capability (CpK)	0.6	1.5	>2	>6
Stock turn	4	19	>25	>50
Manufacturing velocity	0.1%	1%	>8%	>25%
Supply chain costs as % of sales	22%	12%	<9%	<6%
Absenteeism	10%	0.8%	<1%	<1%
Added value per employee	**£10k**	**£200k**	**£400k**	**> £2000k**

This presents a very interesting research challenge for the process control community. ABB is already researching all these areas as a leading first-tier supplier.

Conclusions

This paper tackled the subject of Modeling, simulation ,optimization and control of chemical process with the emphasis on oil and its deviations. In this regard, a common framework was presented in order to decrease the refinery and other related costs and maximizing efficiency. The results of this paper could be useful for all Scientifics and organizations in the field of oil and related industries.

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