# Utilizing Rigorous Simulation in Advanced Process Control projects

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Abstract- Rigorous Simulation helps engineers to understand and identify process dynamics and interactions in a risk-free environment; in addition, it also allows the evaluation and tuning of advanced controllers before they are commissioned. A number of recent APC projects have benefited from this combined methodology, resulting in a better controller design, more accurate inferentials, less plant tests, more confidence with the controller models and an overall reduced risk. Suitability of the methodology for certain units and simulation myths and barriers are reviewed.

#### I. INTRODUCTION

One of the few books that formally describes commercial Model Predictive Control (MPC) technologies dedicates a section to "Some Emerging Technologies for Advanced Process Control: Dynamic Flowsheet Simulation" [1]:

"For more than 20 years, students in process design courses and engineers involved in process design have had as a major tool *steady-state* simulation programs such as FLOWTRAN™, ASPEN™, PROCESS™, HYSIM™, etc. This has removed the drudgery of routine simulation calculations and allowed process designers to test potential design through flowsheet simulation. Unfortunately, until recently, there was nothing comparable available for *dynamic* flowsheet simulation. Individual companies have built ad hoc dynamic flowsheet simulators that have been applied to specific processes to great benefit, but nothing very general was commercially available. More recently, several new packages for dynamic flowsheet simulation have become available. These are listed in the Table – (DIVA, HYSYS, PROTISS, POLYRED, SPEEDUP). Undoubtedly in the years ahead, others will join this list.

Such dynamic simulation packages are essential tools for configuring control schemes that span several units in a flowsheet (e.g., measuring a variable in Unit 2 and manipulating a variable in Unit 1), for studying propagation of upsets and disturbances through a process, for testing control strategies for transition between product grades in a multiproduct plant, and for designing crisis control schemes for handling alarm situations. Clearly dynamic flowsheet simulation will play an important role in the design of future control systems"

The fact is that the Ref. [1] was written in 1994, so the proposition to use rigorous simulation as a tool for process control is not new and the benefits have been clearly identified and documented [2][3][4]. But in today's practice, only a small fraction of process control engineers are common users of rigorous simulation. This requires a more detailed analysis in the following section.

### II. MYTHS AND BARRIERS

There are two types of rigorous simulation: Steady-State and Dynamic. Both can be used in APC projects, but while Steady-State simulation is widely known and adopted by almost all Operating and Engineering companies, Dynamic simulation is still often seen as a difficult and time consuming discipline [5].

Process Engineers are the traditional users of rigorous simulation, primarily Steady-State, since their objective is to design plants at nominal conditions. On the other hand, Control Engineers are focused on maintaining these nominal conditions in a stable and operable state. They should be the true users of rigorous Dynamic Simulation, but due to several myths, they still are not making wide use of dynamic models for their daily work. Let's analyze these myths:

- 1) Lack of mature products: Commercial dynamic simulators were released more than ten years ago. Since then, they have been continuously improved and used for dynamic control and operability studies and for Operator Training. From the product perspective, dynamic simulation is a mature and well-proven technology.
- 2) Requires expert skills: Some dynamic simulators are highly intuitive and interactive, requiring little training. They are conceived to be used by Control Engineers who do not necessarily need to have deep thermodynamic and numerical methods knowledge or computer programming skills.
- 3) Not oriented for Control: Some dynamic simulators include in the standard object palette a complete set of control oriented objects to reproduce almost all basic and advanced control structures, including actual MPC commercial controllers.
- 4) Excessive time for modeling: Ref [6] analyzes modeling efforts from the user perspective. Although the modeling time depends on the process to model and the simulation software used, it has been reduced considerably.
- 5) Requires big computers: Today's commercial simulators are designed to run on standard PCs. Depending on the number of process units included in the model the hardware can still be a constraint, but most of the models used in APC projects do not require large models.

All the above myths are related to the software and hardware used in the simulation, but there are other educational and ownership barriers that are even more important when a control engineer is asked to use rigorous simulation:

- 1) Educational barriers: There is an increasing number of Chemical Engineering universities that incorporate the use of rigorous simulation packages in the academic program, and a subset of those also cover rigorous dynamic simulation. The trend is to include more rigorous simulation content along with existing disciplines such as: Mass and Energy Balances, Thermodynamics, Unit Operations, Process Control, etc, [7]. Dynamic models can be used in the control course to improve understanding of a given process, give students experience in running complex units in real-time, change control configurations and introduce perturbations to the process, thus providing more "real world" experience to the students. But most current control engineers in the process industry have not received education on rigorous dynamic simulation at university, so they still believe most of the myths described above.
- 2) Simulation ownership barrier: Since the first commercial simulation packages ran only in steady-state mode, they were primarily adopted by process engineers. As a result, process engineers became established as the owners and expert users of the simulation packages. When commercial dynamic simulation packages appeared, they were delivered and targeted to the same process engineers, but these engineers found only limited value for their typical process design work, and dynamic simulation was only used for certain dynamic compressors studies or depressuring studies. The historical perception of process engineers as simulation owners (steady-state and dynamic) continues to exclude control engineers from simulation usage. Control engineers can realize the same value from simulations tools as process engineers do for their daily work. Building and maintenance of simulation models should be shared between process and control engineers and both will benefit from their use.

## III. USE IN APC PROJECTS

Deep understanding of the process is the first step in the design of an advanced controller. Control Engineers who implement MPC controllers (usually called Advanced Control Engineers) need to have a deeper understanding of the process and they can benefit from the use of rigorous models [8]. Better integration of the simulation tools and the advanced controllers has resulted in an increasing number of APC projects where simulation tools have been used [9, 10].

Fig. 1 shows the main four phases of an APC project: Pre-test, Plant Test, Detailed Design and Commissioning. Each phase can benefit from rigorous simulation, either Steady-State (SS) or Dynamic (Dyn):

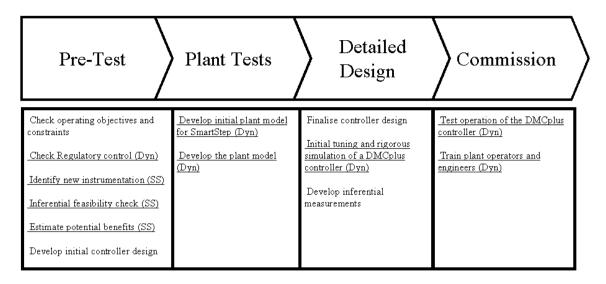


Fig. 1. Use of simulation (underlined) in APC projects.

The first step is to develop a Steady-State model of the unit where APC is envisioned, which in most of the cases is already available in the Process Design department. Then, the model is calibrated to reflect the real plant conditions and, after adding all dynamic data (volumes, valve sizes, k factors, controllers, etc) and setting up the right pressure-flow relations, it can be simulated in dynamic mode using the steady-state data as initialization. The models are then ready to be used in each phase of the project:

1) PRE-TEST: The Steady-State model can be used to estimate the potential benefits of the APC application by specifying in the model a new set of specifications closer to the unit constraints. It is also useful to perform sensitivity analysis to determine optimum location of new instrumentations to identify new instrumentation needs; an example is show in Fig. 2.

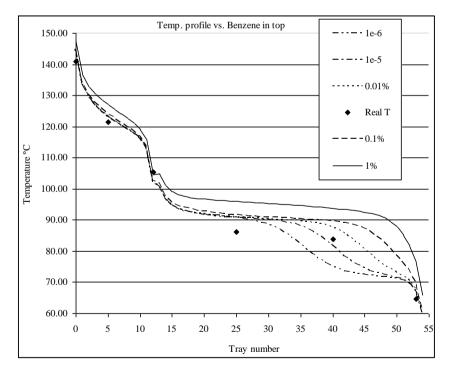


Fig. 2. Sensitivity analysis in Benzene column to identify optimum location for temperature sensor..

The Steady-State models are used to provide input process data for the development of inferentials. The simple inferential methodology is based only in real plant process data as the input for the development of a Partial Least Squares (PLS) model. The inferential methodology based on input data provided by a calibrated rigorous model achieves more accurate and reliable inferentials. For example, Fig.3 shows the same inferential, LGO95% ASTM of a Crude Unit, using both methods: simple and model based.

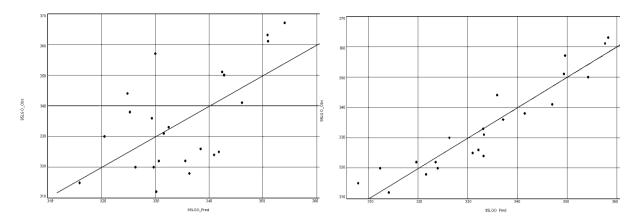


Fig. 3. LGO95% ASTM inferential observed (Y axis) and predicted (X axis) for simple method (left) and model based method (right).

The Steady-State model is also used to determine the non-linearity and the sign gain flip of certain controllers. This is a key element in the development of APC controllers since the MPC algorithms assume the principle of linearity. For example, Fig. 4 shows the benzene contents in the top of a distillation column where a tray temperature is controlled by a basic TC. The controller can be assumed linear for temperatures below 169 Deg C; for higher temperatures the controller flips the gain.

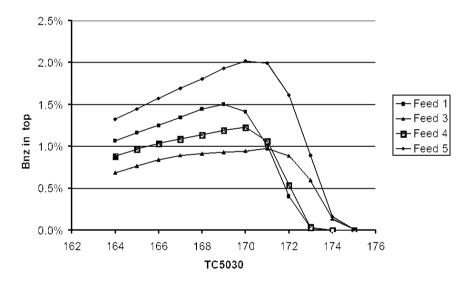


Fig. 4. Benzene content in the top versus controlled temperature in tray section. Gain of TC change sign.

The Dynamic model can be used to check and tune the basic regulatory control system, evaluate alternative control schemes and determine the optimum amplitude of the moves for the plant test.

2) PLANT TEST: Some step tests are applied to the real plant and to the rigorous dynamic model. The step tests performed using the rigorous dynamic model are simple step patterns, and all of them can be performed in less than a day since the dynamic model runs faster than real time. It is important to note that the measured perturbation variables, like air temperature or measured feed compositions, can be included in the step tests of the simulation model. Fig. 5 shows a step test in the dynamic model:

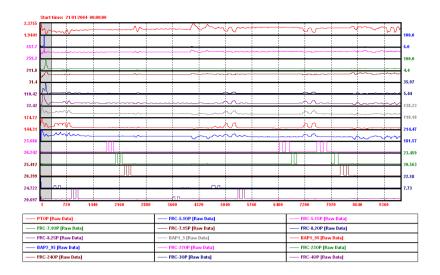


Fig. 5. Results of Step Tests performed over the rigorous dynamic model.

The identified MPC models of the real plant and the rigorous model are then compared and verified, determining where more real Step-Tests are needed. Fig. 6 show comparison of MPC models using real plant step test in an Aromatic fractionation unit and simulation step test:

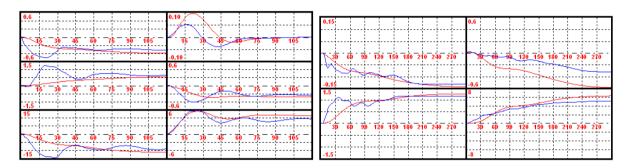


Fig. 6. Comparison of MPC models from real plant [blue] and simulation [red].

If some of the MPC models do not match, it will require a more elaborate analysis for the particular MV-CV couple. The reason for the mismatch can be a poor rigorous model, unmeasured independent disturbances in the real plant, or instrumentation failure, etc. For example, Fig. 7 shows a mismatch for the 17FRC3SP – 17TI82 pair that leads to a revision of the temperature sensor (17TI82), which confirmed a malfunction:

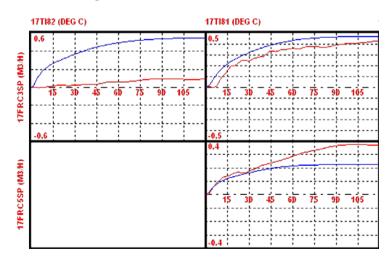


Fig. 7. Left-up corner, mismatch due to instrument failure.

On some units, the Step-Tests can be entirely performed using dynamic simulation, and the identified MPC models can then be used with advanced automatic multitesting packages [11] to fine tune the controller models after a few days of operation.

3) DETAILED DESIGN: The MPC controller need to be tuned and tested, and instead of using the MPC inverted model to tune and simulate the MPC controller with limited model mismatch, the rigorous dynamic model can be used to reproduce all non-linearities and dead times of the process when changing the process conditions or introducing perturbations. The same MPC controller software package and operation interface used for the real plant is linked to the dynamic simulation model.

Processes with long settling times are sometimes difficult to identify, since the plant is influenced by unmeasured disturbances that will contaminate the plant tests. Propylene-propane splitters have settling times of a day or more, and they present challenges in the MPC model identification. The Fig. 8 shows a rigorous dynamic model of a real C3 splitter were the step tests were simulated:

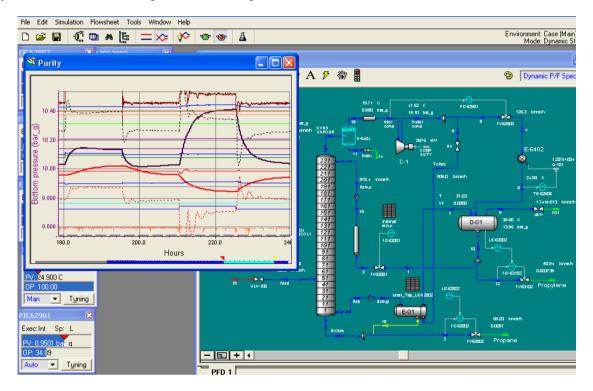


Fig. 8. Dynamic model of a C3 splitter with step test.

Real plant tests were also conducted in the C3 splitter. The Fig. 9 shows the good matching of the identified MPC models from real plant data versus simulation data:

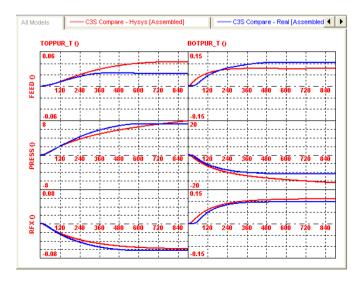


Fig. 9. MPC models of C3 splitter with plant data [blue] versus simulation data [red].

4) COMMISSIONING: Rigorous dynamic simulation provides a much richer model to test the controller in all regimes of operation and different feed compositions. It also provides a rich and risk-free environment to train operators and engineers, being able to reproduce quickly any kind of scenario using the same MPC interfaces that will be used in real plant operation. This is especially interesting for processes with long settling time.

#### IV. BENEFITS AND LIMITATIONS

The benefits associated with the methodology are summarized:

# **Minimize or eliminate Step-Testing:**

- Generate "seed" model for automatic multitest packages
- Calculate optimum amplitude of moves
- Gives confidence with the plant models
- Perturbation moves can be imposed

## Improve and verify MPC controller models:

- Not contaminated by unmeasured disturbances
- Verify linearity range of the process
- Develop better inferentials
- Hidden problems arise when models don not match

# Better testing and training:

- Controller is tested in a wider range of operation
- Basic Control Layout improvements can be quickly studied
- Re-use models for re-testing (revamps or operation mode change)
- Rigorous models available when plant is shutdown or not available
- Rich and risk-free training of operators and engineers

Some processes experience atmospheric disturbances or raw material variations that are difficult to identify in the real plant because they cannot be manipulated and historical data is drowned by other process changes. These variables can be independently manipulated within the simulation.

The time required to develop rigorous dynamic models has always been the main issue for acceptance of this new methodology. The time invested in the development of the rigorous models has to be compensated by the benefits; otherwise it is not worthwhile.

The decision on whether it is practical to use dynamic simulation is determined by the nature of the process, the nature of typical disturbances and the skills of the modeler. Units that show long settling times are those which see maximum benefit from the application of this new methodology. Fortunately, most of these units are based on separation columns, which are quick and easy to simulate, since the thermodynamics packages in leading simulation tools cover most of the required components. For example, C3 splitters, C2 splitters, LNG liquefaction trains, Gas Plants, CDU-VDU, aromatics fractionation, etc are good candidates to consider. On the other hand, reaction units are more complex and this makes them less attractive for dynamic modeling, although the Steady-State models are still valid.

## IV. CONCLUSIONS AND FUTURE WORK

The use of rigorous models in APC projects has been always on the mind of Advanced Control Engineers, but due to historical reasons or myths, this approach has not been used until recently. The increasing adoption of simulation tools by operating companies and the availability of existing rigorous models of the units where APC is envisioned will facilitate the development of the dynamic models, making the methodology more attractive.

One area that will show growth in the future is the development of APC for new plants that have not been built. Engineering Companies design the processes using rigorous simulation models, including detailed dynamic simulations to verify control layouts, safety scenarios and start-up/shutdown procedures. These simulations can also be used to design and prototype APC systems; thus, the correct instrumentation and control layout can be selected from the very beginning to accommodate the needs of a future APC system [12,13]. The main advantage of this approach is the saved time in the final APC phase, where only an update of the MPC models and final tuning is needed. Fig. 8 shows the phases of APC project for a new plant:

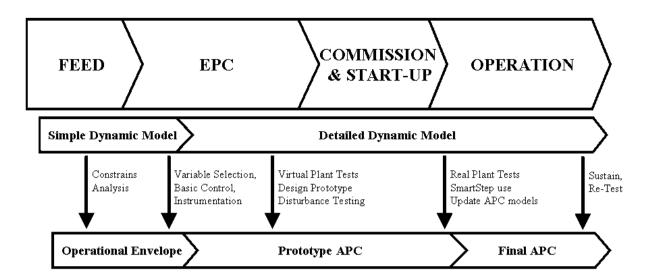


Fig. 10. Prototyping APC in the engineering phase of new plants.

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