# Project design and process control improvements by dynamic simulation of transients

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Although the simulation has been widely employed in chemical and process industries, only during this last decade the steady state approach has been supported by the unsteady analysis and, nowadays, dynamic process models are becoming key tools to improve unit yields and plant stability and controllability. The present paper wants to investigate main benefits in plant design and control coming from the dynamic simulation, above all in terms of safety and economics, and its essential role in the characterization of transients, with the main aim to demonstrate that the unsteady simulation considers solutions often neglected by stationary studies.

## 1. Introduction

In the last years, there has been a considerable improvement in the dynamic simulation, not only in the field of process control, but also in the plant design, preliminary calculations, safety analysis and economic optimization to name a few, through the definition of automatic procedures able to manage plant start-ups and shut-downs (or slow-downs), transients from a steady state to another one or production and quality changes and all those operations which can affect the safety and the economics of an industrial process. In this way, the dynamic modelling becomes fundamental for guaranteeing lower variable costs and for ensuring the achievement of the correct steady state and the required product quality, especially for plants characterized by frequent grade variations or with discontinuous behaviours. Moreover, the support of unsteady analysis allows to ameliorate the start-up procedure in terms of loss prevention, besides the safety of operators, and the implementation of an automatic emergency shut-down (ESD), which consists of sequential actions applicable in case of unexpected emergency situations. The investigation of unsteady conditions using tools based on detailed firstprinciples mathematical modelling can be brought back to the study of Bretelle and Macchietto (1993), on a polymer batch reactor, and to Panthelides and Oh (1996) which adopted gPROMS for modelling a crystallization unit. Subsequently, Gani and Grancharova (1997) solved a differential-algebraic system with the aid of the dynamic

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simulator package DYNSIM<sup>TM</sup>, with a considerable yield improvement and process variability reduction, if compared with the steady state analysis which appears deeply limited if processes characterized by long transients, such as distillation columns or polymer reactors, are considered. More recently, other authors have been used simulation approaches for improving the plant production capacity, i.e. Tremblay (1999), and for developing the plant wide control system on complex chemical processes, Sidrak (2001), sometimes deepening the study till the advanced control feasibility and its possible economic benefits, Manenti and Rovaglio (2005). A general formulation of the problem will be described in the next section and the theory will be applied to a propane/butane splitter, illustrated in the section 3. The main aim is to show through a simple application how the dynamic simulation of transients can assist the process design and improve the control system. The discussion of simulation results will be reported in the section 4.

# 2. Problem Formulation

Dynamic simulators are useful tools for translating chemical processes and unit operations in ODE/DAE systems and integrating them using numerical techniques; different packages for the dynamic simulation exists and everyone is based on a first-principles modelling of unit operations. In any case, a chemical process is frequently represented by the following set of differential-algebraic equations:

$$\begin{cases} \frac{dx}{dt} = f\left(x(t), y(t), p, t\right) \\ 0 = g\left(x(t), y(t), p, t\right) \end{cases}$$
(1)

where x represents differential state vector in the time t, y denotes algebraic state vector and p is a time-independent parameter vector. Differential equations define heat and material balances, whereas algebraic equations ensure thermodynamic, physic and hydraulic properties; nevertheless, the dynamic simulation needs more parameters than a steady case, such as ancillary equipments and geometric dimensions. Moreover, it is necessary to pay particular attention to hold-ups calculations and the tuning of control loops, in agreement with Bezzo et al. (2005).

## 3. Case Study

For showing some important improvement coming from the dynamic simulation of transients, a C3/C4 splitter is modelled in detail and it has been adopted as case study. The depropanizer is fed by a biphasic flow (27% in vapour fraction) which consists of C3, iC4, nC4 and residuals of other hydrocarbons. The feed stream comes from a cryogenic separation system, therefore a preheating is required to increase the temperature till 10 °C. The overhead condenser operates at a medium pressure and low temperature, just beyond 0 °C, that avoid the employment of water as coolant, for refrigerating the vapour stream; instead, the heating fluid supplied to the reboiler is a low pressure steam. The column consists of 10 trays, a reboiler and a partial condenser and it has to ensure two specifications: the first one concerns the summation of iC4 and

nC4 concentrations in the bottom (>98% in mole), whereas the other one imposes the minimization of iC4 and nC4 losses in the overhead gas product. The consolidated control configuration consists of 6 conventional controllers:

- the first loop manages the molar flow fed to the depropanizer;
- the pressure is controlled by a valve positioned on the gas flow exiting from the reflux separator;
- levels of head and bottom vessels are kept constant;
- temperatures of the 1<sup>st</sup> and the 10<sup>th</sup> trays are controlled by regulating the respective utility flow.

Starting from this consolidated control scheme, two different analysis are elaborated: the first one concerns the process design, in particular a variant in the condensation system will be considered, and the second one concerns the process control, analyzing benefits of different conformations at the bottom during the start-up phase.

## 3.1 Alternative project design

The column has to guarantee the butane purity at the bottom, together with the minimum losses of iC4 and nC4 in the overhead flow. With a pressure in the order of 15 atm, for achieving specifications it is necessary to operate around 10 °C in the condenser: that requires the employment of auxiliary fluids as coolant, increasing production costs. Usually, a valid solution involves a second heat exchanger which has the aim to recover energy by interacting with the low temperature of the feed flow. So, in the conformation B (figure 1), the stream exiting from the head of the column crosses a cooler that lowers the temperature below 30 °C using process water. Subsequently, it is further refrigerated in the following exchanger, transferring calories to the feed stream. Moreover, by preheating the feed flow, the requirements of steam consumption in the reboiler is reduced too. The following picture schematizes selected options.

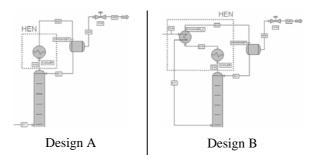


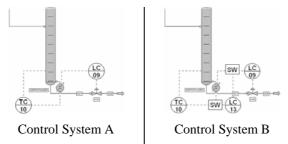
Fig. 1: project design solutions compared in steady and unsteady analysis.

The paper wants to investigate benefits, if they exist, stability and controllability of the configuration A, through the application of the dynamic analysis of transients to the depropanizer, although the stationary study clearly indicates the Design B as the best selection, especially from an economic point of view.

#### 3.2 Process control solutions

The second study wants to testify potentialities of the unsteady analysis in the development of process control systems, comparing performances of different schemes

during the start-up procedure. The classical control system discussed in the previous section ensures the process stability, when the depropanizer operates close to design conditions. Nevertheless, the level controller of the reboiler cannot act during the transient until the required butane purity is achieved, so to avoid off-specs. In this way, a controller which directly acts on the reboiler duty is more efficient and it prevents the partial immersion in the liquid hold-up of the tube side in the reboiler. When quality specifications are reached, it is possible to switch to the classical configuration (sampling of the bottom product). Control systems are reported in the following:



*Fig. 2: traditional (A) and modified (B) process control solutions at the bottom of the depropanizer. The SW is the automatic switch controller.* 

In the Control System B, the LC13 is the unique automatic controller during the start-up and it regulates the heating steam flow for maintaining the liquid level into the reboiler. Only when stationary conditions are almost reached, the automatic control is switched from LC13 to the common configuration, with TC10 and LC09 controllers, that favours the stability of the column at the steady state.

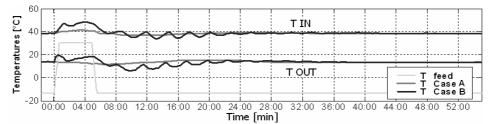
## **4. Simulation Results**

Dynamic models and control configurations implemented in the present study has been performed using the dynamic simulation suite DYNSIM<sup>TM</sup>, a comprehensive, rigorous and field-proven dynamic process simulator for plant engineers, operators and managers, developed by Simsci-Esscor, an operating unit of Invensys System Inc..

## 4.1 Selection of the optimal design

The presence of long transients, internal and external persistent disturbances, grade changes in the production or thermal and material recycle loops in chemical processes is pushing the preliminary design toward an unsteady examination; in fact in such cases, the single stationary analysis is not sufficient in the selection of the appropriate plant design and following pictures want to testify it. Figures 3 and 4 compare trends obtained with the same process control system but different design configurations. In particular, picture 3 shows that the Design B is characterized by a larger range in temperature oscillations after the pulse and how disturbances extend their effect for long time after the perturbation, affecting the process stability; on the other hand, the Design A is able to dampen pulse effects in a shorter time. As a consequence, phase equilibriums and compositions are longer disturbed in Design B. Moreover, in the case B, the required quality is not so easily controllable during transients (figure 4) and the operability

worsens, although a simple pulse is employed. In presence of complex, persistent disturbances, such as fouling/cleanliness factors, the case A only allows the controllability.



*Fig. 3: trends of temperatures across the heat exchangers network in the overhead condenser system (Fig. 1), after 5-minutes-pulse disturbance in the column feed flow.* 

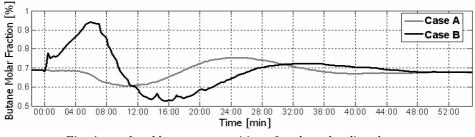


Fig. 4: overhead butane composition after the pulse disturbance.

Even if the stationary study indicates without any doubt the case B as the best design, the unsteady analysis derived from the implementation of a simple disturbance shows how the case A ensure the stability and the operability of the process in a better way and not only: considering the possibility of long transients by using realistic perturbations, the economic losses in off-spec can strongly reduce economical benefits coming from the energy recovery in the Design B.

## 4.2 Control system improvements

Both control systems of figure 2 has been tested during the start-up phase. Controllers TC10 and LC13 are activated in the case A and B respectively, when the reboiler level reaches the setpoint (1.2 m). Then, in the case A, the LC09 is activated when the temperature specification of the TC10 is satisfied; on the other hand, in the case B, when the temperature is near to the TC10 setpoint (which is actually off), the LC13 is deactivated and the control configuration is immediately switched to the traditional system. The figure 5 illustrates the liquid level in the reboiler. When the TC10 is activated in the case A, around the 14<sup>th</sup> minute, the level abundantly overcomes the setpoint and it fluctuates in the range of 0.4 m. With the opening of the overhead reflux valve after 30 min, the level slowly converges to the setpoint. Using the other control scheme, the liquid level is practically flat (variability is in the range of 0.1 m), even if two smaller fluctuations can be observed after 14 min and 24 min: the first one is due to the LC13 lighting and the second one to the reflux activation. At last, the case B halves the start-up duration, from 36 min to 14 min.

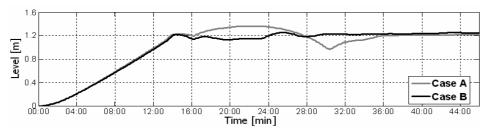


Fig. 5: liquid level in the reboiler during the plant start-up.

The modified control scheme is able to immediately dampen oscillations during the start-up phase, guaranteeing the absence of strong variations in the operating conditions, permitting the turning on of the unit with minimal hold-ups and strongly reducing transient times and risks of undesired phenomena, such as flooding and dumping.

## **5.** Conclusions

The present paper has shown chances to improve design and process control by using the dynamic simulation on a depropanizer. The possibility to simulate expected transients during the preliminary project can be fundamental in the characterization of processes and units, pushing the plant design toward solutions, often discarded or sometimes not even considered in steady state studies. Also in the verification of control systems effectiveness, dynamic simulators appear crucial tools for analyzing which kind of configuration, apart from operating conditions, can guarantee the safety, the operability and the controllability of the plant, besides the respect of environmental regulations and production qualities. Like that, only through a dynamic analysis it is possible to model emergency situations and investigate their feasible solution, reducing damages or, why not, preventing them.

# 7. References

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