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Dynamic Simulation of Chemical Processes and Operational Scenarios to Support the Forensic Engineer

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Detailed dynamic simulation plays an essential role in supporting forensic engineering investigations in industrial accidents, providing the reliable chronological sequence of events and accurately inferring the missing relevant information to reconstruct the puzzle. The case of Texas BP refinery is considered as case study.

1. Introduction

People operating in the field of process systems and control engineering usually ask themselves the question whether the risk of industrial accidents is decreased in the modern plants and production sites. The logic answer should be affirmative since the plant controllability has been strongly improved against some decades ago thanks to the introduction of distributed control system (DCS), model-based predictive control (MPC), and real-time performance monitoring (RtPM) systems (Manenti and Rovaglio, 2008; Lima et al., 2009; Manenti, 2009; Dones et al., 2010). Unfortunately, looking at the practical situation and at the recent disasters, one can easily note that the most relevant industrial accidents happened in these last years in terms of human losses and economic impact as well, in spite of all improvements in process dynamics acquaintance and control. A set of reasons explains this situation. 30-40 years ago, a large-scale refinery processed up to 100,000 barrels of crude oil per day, whereas the current capacity of refineries overcomes the million of barrels per day. It has inevitably taken to many issues dealing with plant controllability. Moreover, if one account even for the more and more frequent integrated process design solutions mainly addressed to energy saving, process intensification, and environmental safeguard, it is easy to realize how plant stability, operability, and flexibility are dramatically limited. To complete the current picture of process industry, it is necessary to mention that some relevant lacks are affecting the operator's knowledge, training, and preparation in managing not only the emergency situations, but also the conventional conditions and the reduced use of operator training simulators (OTSs) has neither decreased the risk of human error nor increased the process understanding of both field and control-room operators. When an industrial accident occurs, the dynamic simulation is more and more an essential tool that cannot be ignored in supporting teams of forensic engineer investigations by

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providing a reliable and unequivocal reconstruction of the accident and a coherent picture of what was wrong so as to define liabilities/responsibilities behind the accident itself. The present research activity is aimed at showing the coupling of forensic investigations and engineering by developing detailed process dynamic simulations. The case simulated and discussed is the reconstruction of the accident occurred at the BP Refinery in Texas City, theatre of an industrial disaster in the March 2005.

2. US Health and Safety Federal Laws

The *Occupational Safety and Health Act* is the primary federal law which governs occupational health and safety in the private sector and federal government in the United States. The Act created the so-called Occupational Safety and Health Administration (OSHA), an agency of the Department of Labor. OSHA was given the authority to both set and to enforce workplace health and safety standards. The Act also created the independent Occupational Health and Safety Review Commission to review enforcement priorities, actions and cases. Only those sections of the Act that are of specific interest are discussed hereinafter (for more details: www.osha.gov/about.html).
Section 5 of the Act contains the “general duty clause”. The “general duty clause” requires employers to 1) maintain conditions or adopt practices reasonably necessary and appropriate to protect workers on the job; 2) be familiar with and comply with standards applicable to their establishments; and 3) ensure that employees have and use personal protective equipment when required for safety and health. OSHA has established regulations for when it may act under the “general duty clause”. The four criteria are: 1) there must be a hazard; 2) the hazard must be a recognized hazard (e.g., the employer knew or should have known about the hazard, the hazard is obvious, or the hazard is a recognized one within the industry); 3) the hazard could cause or is likely to cause serious harm or death; and 4) the hazard must be correctable (OSHA recognizes not all hazards are correctable). Although theoretically a powerful tool against workplace hazards, it is difficult to meet all four criteria. Therefore, OSHA has engaged in extensive regulatory rule-making to meet its obligations under the law.
Section 9 requires that when the Compliance Safety and Health Officer (CSHO) finds violations, with reasonable promptness the employer is notified in writing and this document is called “citation”. Each citation shall describe in detail the nature of the violation, including a reference to the provision of the Act, standard, rule, regulation or order alleged to have been violated. The following points have been found not to excuse untimely notice of contest: misplacement of the citation; manager responsible for OSHA matters went on vacation; demands of ongoing business; lack of experience in OSHA matters; abatement verification form filed during the 15-day period; docketing of the case by the OSHRC's Executive Secretary; belief that correction of violations was sufficient; employer’s financial problems; letter was dated within the contest period, while the postmark was not; telephoning the OSHA area office; oral conversation with a OSHA representative.
Section 11 provides for judicial review: any person adversely affected or aggrieved by an order of the Commission issued under section 10 [Procedure for Enforcement] may obtain a review of such order in any United States court of appeals for the circuit in which the violation is alleged to have occurred or where the employer has its principal

office, or in the Court of Appeals for the District of Columbia Circuit, by filing in such court within 60 days following the issuance of such order a written petition praying that the order be modified or set aside. The findings of the Commission with respect to questions of fact, if supported by substantial evidence on the record considered as a whole, shall be conclusive. Upon the filing of the record with it, the jurisdiction of the court shall be exclusive and its judgment and decree shall be final, except that the same shall be subject to review by the Supreme Court of the United States.
Section 14 deals with representation in civil litigation and provides that except as provided in section 518 (a) of title 28, United States Code, relating to litigation before the Supreme Court, the Solicitor of Labor may appear for and represent the Secretary in any civil litigation brought under OSHA Act but all such litigation shall be subject to the direction and control of the Attorney General.
In case of industrial accident, employers have to demonstrate that all the operators' safety measures have been followed to overcome the presumption of liability incumbent leader to the employers. When accidents happened employers are subject to legal disputes. Normally assurances that employers have stipulated at the beginning of their activities cover any risk and any consequences of accidents, but however employers are involved in legal actions, because employees often start proceedings to claim damages.
These legal proceedings need employers to spend many time and money to defend themselves. Dynamic simulation could anyhow provide a reliable and unequivocal reconstruction of the accident, by giving a coherent picture of what was wrong so as to define liabilities behind the accident itself.

3. Supporting the Forensic Engineer

The forensic engineer has always to face two hard problems. The first deals with the incapability to validate the study on the real plant that has undergone a disaster. The second deals with the limitations of whatever process simulator to properly model industrial accidents (explosions, fireballs, etc) as they are ill-posed problems from a physical point of view (Buzzi-Ferraris and Manenti, 2010). From this perspective, forensic engineering analyses need of two different dynamic simulations: a reduced (simplified) simulation for characterizing those non-conventional situations that brought to the disaster, since these conditions cannot be properly modeled if not by heuristic approaches; a detailed simulation to replace the plant and reproduce the nominal conditions and the dynamics just before the disaster until possible. Detailed simulation is specifically adopted to validate the reduced dynamic simulation. For the sake of conciseness, the simplified simulation only is proposed here.

3.1. Accident Description and Reasonably Detailed Model

The industrial accident here examined has already undergone a series of investigations in the literature (Khana and Amyotte, 2007; Holmstrom et al., 2008). A detailed timetable of events is also available (Holmstrom et al., 2008). As mentioned above, the forensic engineer needs a simplified simulation where no detailed models can simulate non-conventional conditions. Actually, commercial software fails in simulating accident conditions, as no models are able to properly characterize a unit outside their validity range. Thus, as industrial accidents are always related to non-conventional operating conditions, a detailed model is anyway unable to simulate them and the so-called industrial accident simulators are palliative since they may extend a little the model validity range while preserving their limitation to really simulate the system in correspondence with the accident. It is practically impossible to adequately simulate the flooding of a 70 trays splitter where a liquid flow must exit the top of the column just designed for discharge vapor flows. As the splitter was not operating at the accident time, a series of relevant simplifications were assumed to simulate it and we validated them against the detailed dynamic model: as no distillation operations were taking place at the accident point, it is possible to see the column like a large drum that operators were filling and heating; trays and weir volumes were neglected in calculating the effective volume; top condenser and reflux line are negligible for previous assumptions; a 270m-long pipeline is placed downstream the top exit flow to properly account for their pressure drops and time delay; and the blowdown line placed at the bottom is supposed close or however negligible against the flowrate entering the column.

By these assumptions, the overall system can be simulated by means of two interacting drums, one for the splitter and the other one for the blowdown stack (**Error! Reference source not found.**). The feed zone consists of a single stream with assigned molar composition (Khana and Amyotte, 2007): 0.0383 of n-pentane; 0.0263 of 2-methyl-butane; 0.1519 of n-hexane; 0.2950 of 2-methyl-pentane; 0.3072 of n-heptane; 0.1300 of n-octane; 0.0409 of n-nonane; and 0.0104 of n-decane and heavier. The average molecular weight is 93.6 kg/kmol and the density is 649 kg/m^3 at 25 °C. The atmospheric bubble point is 71 °C and the feed flow results liquid. PID1 tuning parameters are $kc=1$ and $ti=0.04s^{-1}$. The column is modeled as a drum with height 52 m and diameter 3.8 m. The only controlled variable is the temperature, which is regulated by PID2 with $kc=0.5$ and $ti=0.01s^{-1}$. The morning of the disaster, the liquid within the column was heated to 150 °C. Pipeline PIP1 is essential to account for pressure drops and time delay between the splitter and the blowdown stack: length is 270 m and internal diameter is 0.35 m. Blowdown stack is modeled using a second drum with a bottom cylinder (diameter 3 m and length 8 m) and a top section (height 26 m and diameter 0.82 m). The geyser of flammable liquid takes place at the top of the stack. The bleed line from the bottom to the sink SNK6 is kept close during the start-up.

4. Dynamic Simulation and Operational Scenarios

Initial conditions and main operations carried out the day of the disaster are implemented. Accident data adopted to validate the simulation is reported in Table 1.

Using all previous information obtained by trivial calculations, an ad hoc scenario involving the following operations has been implemented in DYNSIM (Simsci-Esscor, 2004) so to accurately reproduce accident timetable. All steps of the scenario are sketched hereinafter: (i) Manual configuration of the temperature controller PID2; (ii) The corresponding valve opening XV15.OP is set to zero (no heating at the beginning of the scenario); (iii) The manual valve XV6.OP is completely open; (iv) The manual valve XV14.OP is completely open; (v) Run the accident simulation; (vi) Setpoint PID1.SP equal to 33.11 t/h; (vii) Wait; (viii) Setpoint PID1.SP equal to 84.154 t/h; (ix) Wait; (x) Around 10am the temperature controller PID2 is switched to the automatic mode; (xi) Setpoint PID1.SP equal to 119.55 t/h; (xii) Wait; (xiii) Setpoint PID1.SP equal to 101.59 t/h; (xiv) Wait; (xv) Setpoint PID1.SP equal to 178.81 t/h; (xvi) Wait; (xvii) Setpoint PID1.SP equal to 600 t/h; (xviii) Wait; and (xix) Stop/freeze the simulation. The dynamic trend of some relevant variables during the simulated operational scenario is shown in Figure. Really, the final desired setpoint is unsatisfied since liquid hold-ups of splitter and stack both force the system to stabilize around a flowrate of 150 t/h, which corresponds to the one entering and exiting the stack. When the column is completely filled, the liquid starts entering the stack. After about 6 min 30 s a geyser of flammable liquid is originated. The feed flow is joined to the calculations and the flowrate peak at 4 h 15 min is in correspondence with the total filling of the column and the subsequent filling of the stack. The final mass flowrate setpoint cannot be achieved because of the excessive hydrostatic contribution of column and stack hold-ups.

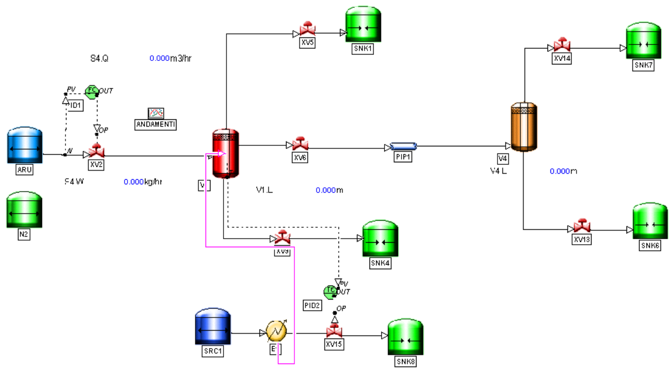

Figure 1. Reduced (simplified) model for the dynamic simulation of the isomerization unit

Time [h:min]	*Holdup [m]*
0	0
0:54	4
2:19	20
3:45	43
4:07	48
4:15	50
4:17	52

Table 1. Liquid hold-up in the splitter

5. Conclusions

Detailed dynamic simulation is more and more a reliable tool to support forensic engineer investigations since it is able to accurately reproduce principal phenomena which lead to the industrial accident. Nevertheless, in correspondence with the accident, operating conditions are always so critical that no detailed models may properly characterize them; actually, fires, explosions, etc., are well-known ill-posed physical phenomena that cannot be properly modeled anyhow. From this perspective, the combination of a detailed simulation and a simplified one gives the forensic engineer the possibility to check with a high accuracy all operating conditions and plant operations before the accident (detailed simulation) and also to rebuilt in an approximate way the accident conditions (simplified simulation) by starting from a reliable operating point that cannot be anymore validated by the field. It is task of the forensic engineer to opportunely simplify the detailed mathematical model by looking at those relevant phenomena that effectively brought to the accident.

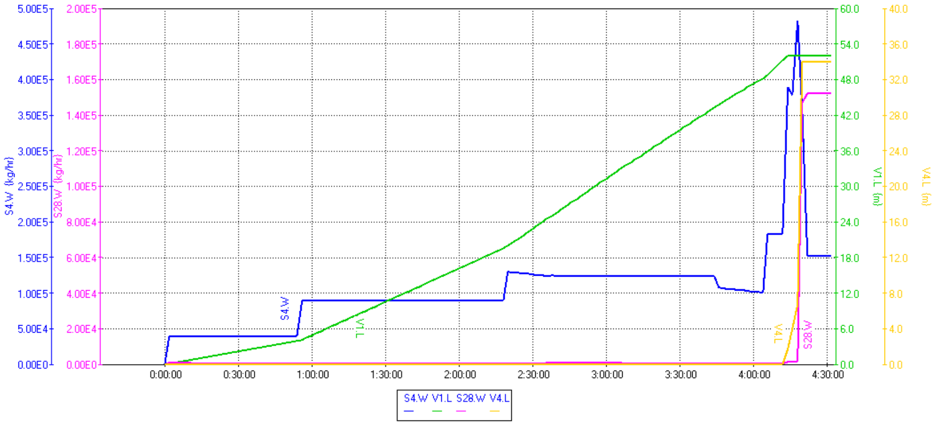

Figure 2. Process dynamics originated by a realistic simulation of the accident: S4.W is the mass flow entering the column; V1.L is the liquid level in the column; S28.W is the mass flow exiting the stack; and V4.L is the liquid level in the stack

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