CHEMICAL ENGINEERING TRANSACTIONS Volume 17, 2009
Editor Sauro Pierucci
 ISBN 978-88-95608-01-3 ISSN 1974-9791
DOI: 10.3303/CET0917051

Dynamic Simulation Of Industrial Accidents

Davide Manca, Sara Brambilla
CMIC Department, Politecnico di Milano
P.zza Leonardo da Vinci, 32 – 20133 Milano – ITALY – davide.manca@polimi.it

In the past, process simulators and accident simulators belonged to two distinct worlds. Dynamic process simulators were mainly applied to process control, process dynamic investigation and safety analysis (in terms of definition of emergency shutdown procedures). Accident simulators were related usually to the steady state accident investigation, as well as risk analysis and emergency preparedness and response. The manuscript shows how the coupling of process and accident simulators represents an innovative and powerful tool to support the engineer's activity in several fields, *e.g.* process planning, process control, accident investigation, accident preparedness and response. The biunique interaction between these simulators allows investigating feedbacks and interactions among plants and industrial accidents. Actually, process dynamics affects the source term, *i.e.* the amount of released components and their chemical and physical properties, while the accident dynamics closes the loop by affecting the plant dynamics. The accident may have a direct effect on the plant dynamics (as in the presence of a heat source, *e.g.* a pool fire) or may have an indirect effect by influencing the integrity of field operators when the release of a toxic substance occurs. The manuscript shows the biunique interactions between a pool fire (originated by the release of a flammable liquid, as the consequence of an industrial accident) and the process itself.

1. Introduction

Dynamic process simulation has become an indispensable and central tool for process design, analysis, and operation in the chemical industry. The dynamic simulation of a chemical process is a step ahead from the steady state analysis and has some effective and significant advantages. A dynamic simulation of the process allows: checking the control system configurations before applying it to the real plant so as to uncover possible control system errors; training the operators to increase their awareness and skills; planning and testing the start-up and shutdown procedures; increasing the process safety by testing and validating the procedures in a non-destructive environment. The support of a dynamic process simulator to training allows operators gaining experience, facing malfunctions and deviations from the nominal conditions, and becoming aware of the importance of following the correct procedures. The operators can modify virtually the process variables of the dynamic simulation while quantifying the consequences on the plant conditions without incurring into real risks.
Moreover, the operators are trained to cope with plant deviations from nominal conditions due to accidental events that affect either the plant (*e.g.* emission, release, fire, explosion) or the people working in the plant (*e.g.* a fire, explosion, toxic gas cloud). Industrial accidents are dynamic phenomena that evolve depending on the

Please cite this article as: Manca D. and Brambilla S., (2009), Dynamic simulation of industrial accidents, Chemical Engineering Transactions, 17, 299-304 DOI: 10.3303/CET0917051

environmental conditions and the characteristics of the emitted substance or mixture. Consequently, to simulate a realistic unusual situation in case of accident, both the dynamics of the plant and of the accident should be accounted for and run simultaneously, since they are interrelated and mutually influenced. For instance, process conditions determine the leakage characteristics whilst accident consequences affect the plant variables.

2. Integration of Process and Accident Simulators

To evaluate simultaneously both the process condition and the accident evolution it is necessary to link the chemical process simulator to the accident simulator. Both the accident and the process dynamics should be simulated in a CPU time that allows achieving a real-time performance. Furthermore, the simulation should be so responsive to perform simulations faster than clock-wall so to shorten the dynamics of transients and catch the attention and participation of operators.

On the side of process simulators, DYNSIM® (Simsci-Esscor, 2006) meets these prerequisites (in fact, it is used for Operator Training Simulation).

With reference to accident simulation, there is no commercial software based on a single and *unified* model capable of modeling and simulating interconnected and consequent events, *e.g.* emission → spreading → evaporation → ignition → fire → dispersion. Actually, there are a number of programs that simulate only some of the aforementioned events and ask the user to specify some input data that can be computed by other software. These programs force the user to pass manually the output of a program to the following one as input data. In addition, it is still missing an automated procedure that links the single pieces of software to get the whole picture of the accidental event. Finally, the commercial software was coded for direct and interactive used by means of a GUI (graphical user interface). This software neither is designed to be interrogated and run automatically by another program nor is it designed to exchange data biuniquely with another program. For all these limitations and weaknesses we chose to develop AXIM™ a proprietary code meant to meet the previous specifications.

AXIM™ is not based on Computational Fluid Dynamics (CFD) models since they are still not practicable for real-time response. Conversely, AXIM™ adopts, implements, and in some points improves a number of well-known models in the literature. Moreover, some features are original of AXIM™, to cite only the most important the dispersion of heavy gases in complex environments such as industrial plants. The most important literature models implemented in AXIM™ are the spreading and evaporation of liquid pools (Brighton, 1985; Webber and Brighton, 1986; Webber, 1987, 1990, 2000; ABSG Consulting, 2004), and the pool fire dynamics (McCaffrey, 1979; Rew and Hulbert, 1996; Engelhard, 2005; Fay, 2007; Raj, 2006, 2007a, 2007b). Brambilla and Manca (2009) report more details on the features of AXIM™.

DYNSIM® and AXIM™ are based on two distinct differential algebraic equation systems. At each integration step, a set of process variables is passed to and fro the simulators.

Let us suppose that the objective of the coupled simulation is evaluating the consequences produced by a pool fire on an industrial plant. DYNSIM® computes and passes the flow rate and temperature of the released substance to AXIM™. Afterwards, AXIM™ evaluates the heat radiated to the equipment surrounding the pool fire and passes it to DYNSIM®. At each integration step, the simulators share some piece of information. To accomplish this task, there is need for an ad-hoc interface to make feasible the communication between the simulators. It is worth underlining that the

availability of the source code of AXIM^{TM} allows linking it to any other dynamic process simulator such as Aspen HYSYS®, Aspen Plus®, Unisim®. According to the software, the link can be based for instance on the OPC (OLE for Process Control) protocol, DLL (Dynamic Link Library), CIO (compiled interconnection objects).
During the synchronized time-steps, AXIM^{TM} assumes that the input variables from the process simulator (*e.g.* release flow rate and temperature) are constant. The same happens for the process simulator with the variables it receives from AXIM^{TM} (*e.g.* heat radiated to the equipment surrounding the fire). Therefore, it is advisable to pay attention when selecting the time interval between two calls of these simulators. It should be neither too short, to avoid excessive CPU times, nor to long, to avoid major discrepancies between the simulated and real dynamics.

3. Accident Simulation

We focus our attention on a possible industrial accident in the supply section of a toluene hydrodealkylation to benzene plant (Douglas, 1988). The accidental scenario involves the formation of a hole in the pipe that transfers toluene from the storage to the reaction sections. Since toluene is stored at ambient temperature and pressure, the liquid released from the hole does not flash and forms a pool on the concrete ground. DYNSIM® simulates the hole with a lower flow rate reaching the reactor. The liquid flow rate spilled from the hole may change in time according to the dynamics of process variables (*e.g.* the pressure inside the pipe) or to deliberate actions (*e.g.* the closure of an emergency valve on the feed line). AXIM^{TM} computes the pool dynamics, *i.e.* the pool radius and height, the evaporation rate, and the pool temperature.
A spark ignites immediately the gas that evaporates from pool, and causes a pool fire. The pool fire is described in terms of a tilted elliptical cylinder characterized by a larger diameter in the wind direction, due to the wind-exerted drag (Brambilla and Manca, 2009). The accident simulator evaluates the flame diameter, the flame height, and the surface emissivity. By combining these data with the position and geometry of the equipment surrounding the flame, it is possible to compute the heat radiated to the surrounding process units. The radiative heat is an incoming heat source for the units and modifies their process conditions. With reference to the sub-cooled toluene, the radiated heat affects mainly the process temperature. The effect is bigger for batch process units and smaller for continuous units, due to the enthalpy flux conveyed by the liquid flow. It is worth underling that the larger the amount of liquid stored in the equipment, the lower the temperature increase. Therefore, as the dynamic process simulator computes the spillage conditions and the modification of plant operation due to the additional incoming heat flux, the accident simulator determines the heat radiated to the surrounding equipment. The data are exchanged biuniquely and dynamically.
This case study assumes that the conventional control system is not able to control the erratic behavior of the process once the accident has occurred. Consequently, the control room operator has to select the proper emergency shutdown procedure by either opening a safety valve or cutting off the inlet flow rate. At the same time, the field operator should pay attention to both heat radiation and toxic release threshold when he monitors at a safe distance the pool fire dynamics.

4. Numerical Results

The case study assumes that, before the accident occurs, the plant is in steady-state conditions. An unpredictable accident forms a hole into a pipe and the emitted toluene spreads onto the concrete ground. A spark suddenly ignites the pool and a pool fire develops and radiates a time-varying heat to the surrounding equipment according to the flame dimensions (diameter and height), the burning rate, and the atmospheric and wind conditions.

We evaluated the accident consequences on an intermediate small process drum and a larger storage tank. The former is representative of a continuous unit, while the latter of a semi-batch unit. The intermediate process drum supplies the toluene flow rate to the broken pipe.

Table 1 reports the geometric data of both vessels. "Distance" is the space between the centers of the flame and of the process units.

Table 1: Geometrical features of the process units influenced by the pool fire.

Process unit	Diameter [m]	Height [m]	Distance [m]	Liquid level [m]
Process drum	1	2.5	4	0.5
Storage tank	6	5	10	3.0

The process simulator determines the liquid flow rate that is spilled from the hole and changes dynamically due to variations the pipe pressure and deliberate actions (*e.g.* the closure of an emergency valve on the feed line). We assumed the flow rate to be constant (*i.e.* 0.8 kg/s) due to the presence of a process pump. In the meantime, the accident simulator computes the liquid pool and pool fire features, and quantifies the pool and flame dimensions. From the plant geometry, the accident simulator determines the view factors between the flame and the surrounding process units and the impinging radiation. Therefore, while the dynamic process simulator evaluates the liquid flow rate and the modification of plant conditions due to the unexpected incoming heat flux, the accident simulator determines the amount of heat radiated to the surrounding equipment. The data are exchanged biuniquely and dynamically at predefined intervals.

The case study assumes that the control-room operator perceives the occurrence of the accident after 10 minutes and then he/she alerts the field-operator, asking for a prompt intervention by physically closing the upstream emergency valve to intercept the flow from the intermediate process drum. Eventually, the leakage ceases and the pool fire extinguishes rather quickly according to the burning rate (0.066 kg/m2 s).

Figures 1 and 2 show the effects of the pool fire on the process drum and on the storage tank in terms of temperature variations and radiated heat. When a spark ignites the pool both the equipment temperatures start increasing. A higher temperature derivative corresponds to higher values of flame radiation, which occur in the first 30 seconds. After some minutes, when the burning rate almost compensates the incoming liquid flux, the pool fire reaches a pseudo-steady-state condition, and the temperature derivative decreases. Finally, when the upstream emergency-valve is closed and the liquid spill is over, the radiative flux rapidly extinguishes.

The temperature increase of the storage tank is negligible due to the high thermal inertia. Actually, this tank contains 73 tons of toluene that has a heat capacity of 1700 J/kg K, and the average dose is 20 kW, corresponding to a temperature derivative of 1.5×10^{-4} K/s. Conversely, despite the inlet flowrate to the process drum is 10 kg/s, the temperature increase is much higher (about 7 K) because the drum is closer to the flame and receives a higher thermal radiation.

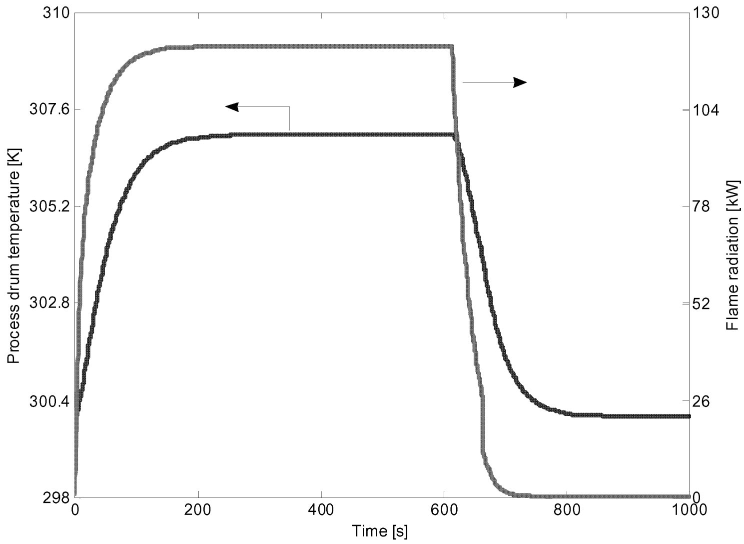

Figure 1: Influence of the pool fire on the intermediate process drum

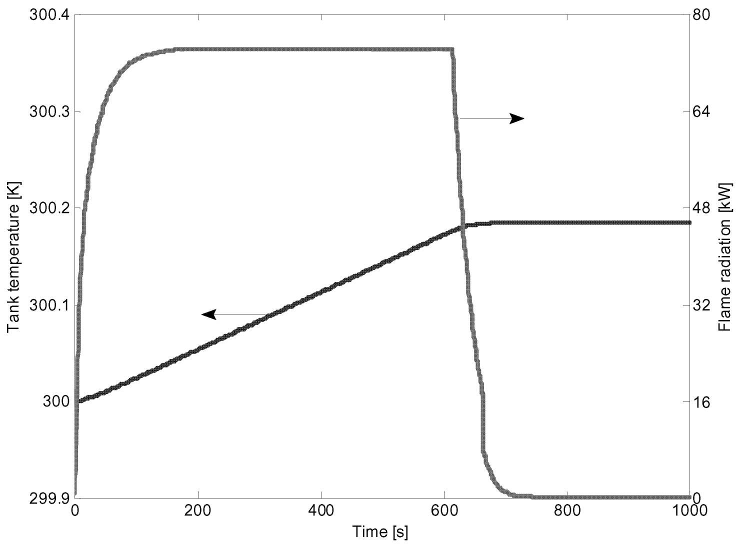

Figure 2: Influence of the pool fire on the storage tank

The temperature of the process drum returns faster to the steady state when the flame extinguishes. This is due to the small material inertia and the flow of the toluene. The toluene flow rate emitted by the hole in the pipe varies for less than 4% during the 10 min spillage, because the process drum pressure is not much influenced by the temperature increase. In fact, toluene is a high-boiling liquid (383.8 K) and its vapor pressure is rather low at the temperatures reached during the accidental event. These bits of information are quite important for the training of both control-room and field operators.

5. Conclusions

The dynamic analysis performed in this manuscript demonstrated that an industrial accident may affect the plant behavior, making it deviate from nominal operating conditions. In particular, the effect of a pool fire onto two vessels was investigated and discussed. An increase of both temperature and pressure was observed. As far as the accidental outcomes are concerned, the liquid spread and burning determined the flame shape (*i.e.* diameter and length). We quantified the magnitude of the interaction between the process and the accident, highlighting that it valuable for risk-assessment and for control room and field operator training.

References

ABSG Consulting Inc., 2004, Consequence Assessment Methods for Incidents Involving Releases from Liquefied Natural Gas Carriers, for the FERC (Federal Energy Regulatory Commission) under contract number FERC04C40196.

Brambilla S. and D. Manca, 2009, Accidents Involving Liquids: a Step Ahead in Modeling Pool Spreading, Evaporation And Burning, Journal of Hazardous Materials, 161, 1265–1280.

Brighton P.W.M., 1985, Evaporation from a Plane Liquid Surface into a Turbulent Boundary Layer, J. Fluid Mech., 159, 323-345.

Douglas J., 1988, Conceptual Design of Chemical Processes, McGraw-Hill, 1988.

Engelhard W.F.J.M., 2005, Heat flux from fires, in: Methods for the Calculation of Physical Effects due to Releases of Hazardous Materials (Liquids and Gases), Ed. van der Bosch C.J.H., Weterings R.A.M.P, Netherlands.

Fay J.A., 2007, Spread of Large LNG Pools on the Sea, Journal of Hazardous Materials, 140, 541-551.

McCaffrey B.J., 1979, Purely Buoyant Diffusion Flames: Some Experimental Results, Center of Fire Research, NBSIR 79-1910.

Raj P.K., 2006, Spectrum of Fires in an LNG Facility. Assessments, Models and Consideration in Risk Evaluations - Final Technical Report, Contract Number: DTRS56-04-T-0005.

Raj P.K., 2007a, Large Hydrocarbon Fuel Pool Fires: Physical Characteristics and Thermal Emission Variation with Height, Journal of Hazardous Materials, 140, 280-292.

Raj P.K., 2007b, LNG Fires: a Review of Experimental Results, Models and Hazard Prediction Challenges, Journal of Hazardous Materials, 140, 444-464.

Rew P.J., Hulbert W.G., 1996, Development of a Pool Fire Thermal Radiation Model, HSE Contract Research Report n. 96/1996.

Simsci-Esscor, 2006, Dynamic Simulation Suite User Guide, http://www.simsci esscor.com.

Webber D.M., P.W.M. Brighton, 1986, Inviscid Similarity Solutions for Slumping from a Cylindrical Tank, Transaction of the ASME, 108, 238-240.

Webber D.M., 1987, Heat Conduction Under a Spreading Pool, SRD R421.

Webber D.M., 1990, A Model for Pool Spreading and Vaporization and its Implementation in the Computer Code G*A*S*P, AEA Technology, SRD/HSE/R507.

Webber D.M., 2000, Model for Pool Spreading, Evaporation and Solution on Land and Water (PVAP) – Verification Manual, in PHAST 6.0 Manual.