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DYNAMIC SIMULATION OF INDUSTRIAL ACCIDENTS

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In case of a chemical accident in an industrial facility, the properties of the release (*e.g.*, flow rate, liquid and vapor fractions, temperature, and momentum) may vary in time due to the modifications of the conditions inside the process unit ascribable to the leakage itself and/or to the intervention of either the operator or the control system. This manuscript describes an effective methodology and the features that an accident simulator should implement to account for the release variability. In particular, the paper focuses on accidents involving the release of liquids, their spreading, and the formation of pools.

The recommended features include the capability to simulate the automatic switch of the liquid pool from spreading to shrinking, its vanishing, the release in a bund, the ignition of the evaporating vapors, the evaluation of the pool-fire geometrical dimensions and view factors, and the evaluation of the heat fluxes radiated to the surrounding equipment and field operators. By implementing these features in an accident simulator, it is possible to get a more realistic picture of the accident evolution, and of its magnitude and consequences, especially when the process and the accident influence each other.

These features have been implemented in a simulation program, AXIM™, which is based only on CPU-efficient models and algorithms to simulate the accidental scenario faster than the real accident. This characteristic allows linking the accident simulator to a dynamic process simulator that evaluates the real conditions inside the process units, by considering the material, momentum, and energy balances.

The possibility to develop an advanced OTS is also investigated.

Keywords: Dynamic accident simulation; Chemical accidents; Operator training simulation; Pool spreading, evaporation, and burning.

1. IDENTIFICATION OF THE PROBLEM

Since large quantities of potentially hazardous substances are handled, stored, processed, and transported worldwide (*e.g.*, crude oil derivates, ammonia, chlorine), it is highly desirable to adopt high safety standards by a proper design, management and control of plants, transport systems, and storage sites in order to avoid or at least mitigate the outcomes of possible chemical accidents. In fact, chemical accidents lead to dramatic consequences, such as the loss of lives among field operators, responders, and population; and the discharge of toxic and/or flammable substances in the environment. In addition, chemical accidents entail costs for both the company, liable for the accident, and the surrounding community due to reconstruction costs, loss of production, court costs, fines, business interruption, reallocation of production to other sites, cost of on site personnel and contractors, plant redesign, and costs for the civil and health authorities (Fewtrell and Hirst, 1998).

Stakeholders have the primary role and responsibility respect to accident prevention, preparedness and response. Hazard identification and risk assessment are necessary for an extensive understanding of possible risks to operators, citizens, environment, and property. A hazard analysis allows identifying the risks associated to hazardous chemicals so to intervene selectively to mitigate or eliminate them. It would be preferable if the hazard identification and risk assessment were undertaken from the earliest stages of design and construction, by addressing the causes of human and technological failures, as well as the accidents that can be originated by natural disasters or deliberate acts (*e.g.*, terrorism). Once the hazard analysis has

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identified the top events, there are a number of computer programs available in the literature and on the market that quantify and characterize the accidental scenarios to support the actions and decisions of the subjects involved, at different levels, in the emergency preparedness (*e.g.*, civil authorities, rescue teams). The simulation of chemical accidents is an important element of the hazard analysis. The paper analyzes and discusses the features that an accident simulator should implement to get a more realistic simulation of the accident consequences. Section 2 discusses a different approach to the simulation of industrial accidents; Section 3 discusses the feature of a dynamic accident simulator (AXIM™); Section 4 illustrates the interactions and feedbacks between a dynamic process simulator and a dynamic accident simulator; and Section 5 shows a case-study.

2. A DIFFERENT USE OF ACCIDENT SIMULATORS

A hazard analysis identifies the possible accidents and their simulation allows assessing their impact on the surrounding process units, the people, and the environment. As far as the accidents occurring in chemical industries are concerned, a further step towards increasing safety can be achieved by considering that the accident dynamics is influenced by the evolving conditions of the damaged process unit. These conditions may vary because of:

1. the intrinsic phenomenology of the release (*e.g.*, the liquid flow rate from a hole in a tank depends on the liquid head, which decreases progressively if no liquid is added to that tank);
2. the material, momentum, and energy balances across the process units;
3. the intervention of the control system or operators (*e.g.*, by closing a valve it is possible to cut off the flow to a broken pipe, and interrupt the release);
4. the feedbacks from the accident.

Points 2, 3 and 4 usually are not implemented in common existing software like ALOHA™ (Reynolds, 1992), EFFECTS (TNO, 2007), and PHAST (DNV, 2007). Nonetheless, to get a more realistic picture of the accident dynamics, especially when the control system intervenes to safeguard the plant and the production, it is necessary to include points 2 and 3 in the simulation of the accident. This can be accomplished by evaluating the behavior of the process and of the control system with a dynamic process simulator, *e.g.*, Aspen HYSYS™ (AspenTech), DYNSIM™ (Simsci Esscor, 2006), UniSim® (Honeywell, 2008).

Point 4 underlines the fact that the conditions of the plant may modify due to the feedbacks from the accidental event as it may happen in case of fire, when the heat flux radiated towards the surrounding process units modifies their temperatures and may melt the cables that are not fire proof so limiting the possibility to intervene of the control system. This issue can be taken into account by linking a dynamic process simulator to a dynamic accident simulator to exchange data biuniquely. In this context, the accident simulator is connoted by the adjective “dynamic” to stress its capability to account for variable input data, whose variability is unpredictable since they depend not only on the conditions of the damaged process units but also on the intervention of both the control system and the operators.

The simultaneous evaluation of the conditions of the process and the accident, as well as their feedbacks is a promising and advisable feature to get a more realistic picture of the accidental event while assessing the effectiveness of the emergency measures and procedures.

This coupling represents also an effective tool for training the operators, *i.e.* it can be used as an advanced Operator Training Simulator (OTS). Conventional OTSs are based mainly on a dynamic process simulator, *i.e.* a simulator that can describe the non-stationary evolution of the plant when some disturbances occur, and can investigate the process conditions. The advanced OTS would be dedicated not only to the training of operators within a virtual plant, where they can modify the process variables while quantifying the consequences on the plant conditions without incurring into any real risks or compromising the production, but also to their training at coping with accidental events, such as leakages. In this case, the dynamic accident simulator would evaluate the accidental consequences, which are influenced by the emergency procedures implemented by the operator. With the advanced OTS, the operators are expected to gain experience on the process, and to get used to face malfunctions and deviations from nominal conditions, and to cope with accidents. In addition, the coupling between the accident and the process dynamics allows testing the effectiveness of mitigation systems, and emergency procedures to shutdown the plant.

In order to build an OTS for the simulation of industrial accidents, the process and the accident simulators must be coupled into a real-time tool, so that the operators become aware of the time scales of the occurring phenomena. In addition, the accident simulator must implement the "dynamic" feature to deal with unpredictable input data that cannot be evaluated from aprioristic considerations on the process variables since they depend on the dynamic evolution of the process.

Section 3 gives an overview on a program for the simulation of the chemical accident (AXIM™, Brambilla and Manca, 2009a) that can account for the unpredictable variability of the source term.

3. AXIM™ OVERVIEW

AXIM™ is an accident simulator that can be run either as a standalone program (*e.g.*, for risk analysis, risk assessment, emergency planning) or as a software module (*i.e.* DLL – Dynamic Link Library, OBJs – compiled object files) called by another program (*e.g.*, an operator training simulator, a dynamic process simulator, a platform for industrial accident simulation). At present, AXIM™ (Brambilla and Manca, 2009a-b; Brambilla, 2009) can simulate the dispersion of pure substances in the environment. Most of the input data (*i.e.* meteorological conditions, date, computation domain, surface, targets, bund, and ignition source presence) can be assigned by the user through a graphical user interface that increases significantly the usability of the program and avoids the input of inconsistent data. Conversely, the data related to the source term can come in part from the dynamic process simulator. For instance, the hole size and position within the plant needs to be defined by the user in the graphical user interface, while the emitted flow rate is evaluated by the dynamic process simulator.

As far as the release of a liquid is concerned, AXIM™ accounts for the spread of the emitted liquid on eight different typologies of surfaces: open water (*i.e.* sea), isolation concrete, light concrete, heavy concrete, average subsoil with 8%wt of moisture, dry sandy subsoil, wet sand with 8%wt of moisture, and gravel bed. The database includes information related to the physicochemical properties of these surfaces (density, specific heat capacity, thermal conductivity, thermal diffusivity, and kinematic viscosity, this last only for water), and their reflectivity, moisture content, and average surface roughness.

The physicochemical properties of the emitted substance are evaluated according to the DIPPR database (DIPPR, 2004). In particular, the accident simulator uses the molecular weight, critical pressure, critical temperature, boiling temperature, melting temperature, heat of combustion, latent heat, compressibility factor, adiabatic constant, material diffusivity, vapor pressure, reflectivity of the liquid phase, surface tension, lower and upper flammability limits, density, specific heat capacity, thermal conductivity, material diffusivity, and dynamic viscosity. Some properties are evaluated for both the liquid and the vapor phases.

To account for the source term variability, the accident simulator includes the capability to simulate:

- the automatic switch from spreading to shrinking of a liquid pool, its evaporation and vanishing;
- the release in a bund;
- the ignition of the pool;
- the evaluation of the geometrical dimensions and view factors of the pool-fire, and the quantification of the radiative heat flux emitted to the surrounding equipment and field operators.

4. COUPLING OF THE DYNAMIC PROCESS AND ACCIDENT SIMULATORS

Coupling the dynamic simulators of chemical process and accidental events has the aim to evaluate simultaneously both the process conditions and the accident evolution. This is important when the accident consequences affect the plant, *e.g.*, when a fire occurs. While liquid pools or gas releases do not influence directly the plant, a fire is a heat source that radiates the surrounding process units, structures, and operators, and can lead the process to deviate from the standard operating conditions. To achieve the aforementioned coupling, both the accident and the process dynamics should be simulated in a negligible CPU time to get an almost real-time performance.

There are some tangible benefits deriving from the interaction of a process simulator with an accident simulator. First of all, a trainer can adopt this tool to supervise the activities of trainees, by judging the operator's knowledge of procedures, the response to unusual situations, as well as his/her human and technical reliability. As far as accident investigation is concerned, the aforementioned software coupling allows examining and understanding the accident dynamics, so to implement the most effective mitigation measures and/or prevent them. Moreover, the accident simulator allows analyzing the system vulnerabilities while identifying the appropriate corrective actions. This tool is also useful under emergency preparedness to better plan the emergency response.

The proposed integration between a process dynamic simulator and an accident simulator is not only powerful from both a technical and a safety point of view, but allows also assessing the human factors issue. In fact, from a safety management perspective, the data gathered on the behavior of operators when simulating the plant management under emergency conditions are much more revealing than a desk exercise on emergency response.

From the technical point of view, at each integration step, some process variables are passed to the accident simulator and *vice versa*. Let us suppose that the objective of the coupled simulation is evaluating the consequences of a pool-fire in an industrial plant (see Section 5 for a quantitative analysis). The dynamic process simulator computes and passes to the accident simulator the flow rate and temperature of the released substance. On the other hand, the accident simulator evaluates the heat radiated to the equipment surrounding the pool-fire and passes it to the process simulator. Thus, at each integration step, the simulators have to share some pieces of information. To accomplish this task, there is the need for an *ad-hoc* interface to make feasible the communication between the simulators.

During the time-step, the accident simulator assumes that the variables it receives from the process simulator (release flow rate and temperature) are constant. The same happens for the process simulator with the variables it receives from the accident simulator (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. We chose to adopt a time-step of 0.5 s.

5. CASE-STUDY: FORMATION OF A TOLUENE POOL-FIRE

This section discusses a specific case-study to illustrate the biunique interactions between a chemical process and an accident. The case-study does not refer to any accidents happened in the past. However, it is noteworthy because, despite its simplicity, it clarifies the complexity and advantages of the risk assessment technique based on the simultaneous simulation of the plant and of the accident dynamics.

The scenario refers to the supply section of the plant for hydrodealkylation of toluene to benzene plant (Douglas, 1988; Luyben *et al.*, 1998). The virtual accident consists in the formation of a hole in the pipe that transfers the toluene from the raw material storage site to the reaction section. The toluene is at ambient temperature (see Figure 1).

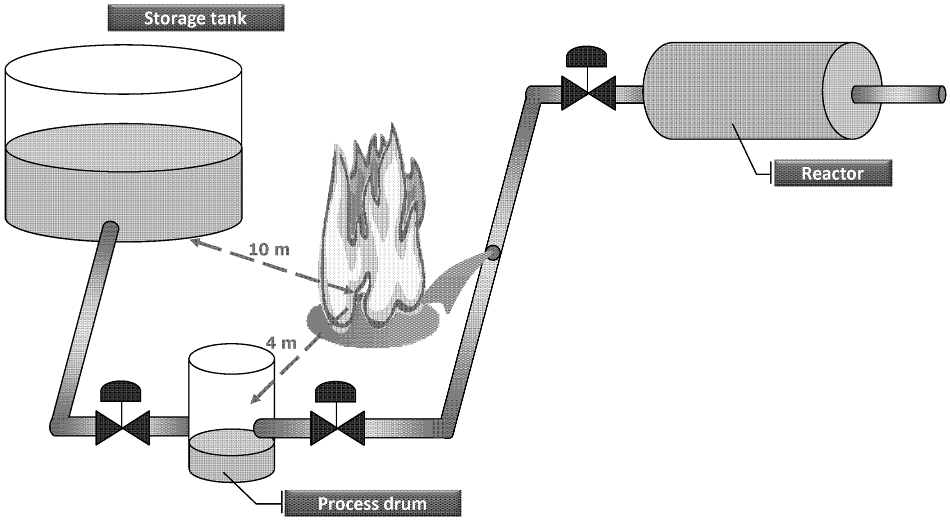

Figure 1: Schematic layout of the process and of the accident

The liquid spilled from the hole forms a pool on the concrete ground that is ignited when it reaches a radius of 2 m. The process units near the flame receive a radiative heat flux that may modify the operating conditions, *i.e.* the temperature. The expected effects are more relevant for both batch equipment and storage tanks, whilst they are more reduced for continuous units, due to the enthalpy flux conveyed by the liquid flow. In addition, it is worth underling that the larger the amount of liquid stored in the unit, the lower the temperature increase (under the same incoming radiative heat).

The case-study assumes that the conventional control system is not able to detect automatically the leakage in the pipe. Consequently, the control room operator has to select and implement a proper emergency procedure. In this case, the operator should stop the pump that transfers the toluene from the intermediate vessel to the reaction section in order to cut off the outflow from the pipe and the operator should switch off the pump feeding the intermediate vessel. At the same time, he/she has to close the valves to isolate the damaged pipe section.

We assumed that the accident affects mainly an intermediate vessel and a larger storage tank. The former is a continuous unit, whilst the latter is a semi-batch unit. The intermediate vessel supplies the toluene to the broken pipe.

Table 1 reports the geometric features of the process units.

Table 1: Geometric data of the process units near the pool-fire

Process unit	Diameter [m]	Height [m]	Fire-proc. unit distance [m]	Liquid level [m]	Liquid holdup [m^3]
Intermediate vessel	1.0	2.5	6	0.5	0.4
Storage tank	6.0	5.0	10	3	84.8

Since the storage tank holdup is two-hundred times larger than the intermediate vessel holdup, we expect that its temperature will experience a lower increase in the liquid temperature.

We assumed that the control-room operator becomes aware of the accident 15 min after the formation of the hole. Consequently, the operator switches off the pumps. At that point, the intermediate vessel is isolated from the plant and behaves as a batch unit. The flame diameter is larger than the pool diameter because of the drag exerted by the wind. The quasi-steady state from about 400 to 900 s occurs when the emitted flow rate equals the burning rate. During the release, the dynamic process simulator determines that the leakage varies linearly from 22.7 kmol/h to 23.6 kmol/h.

Figure 2 shows the dynamics of both the pool and fire diameters.

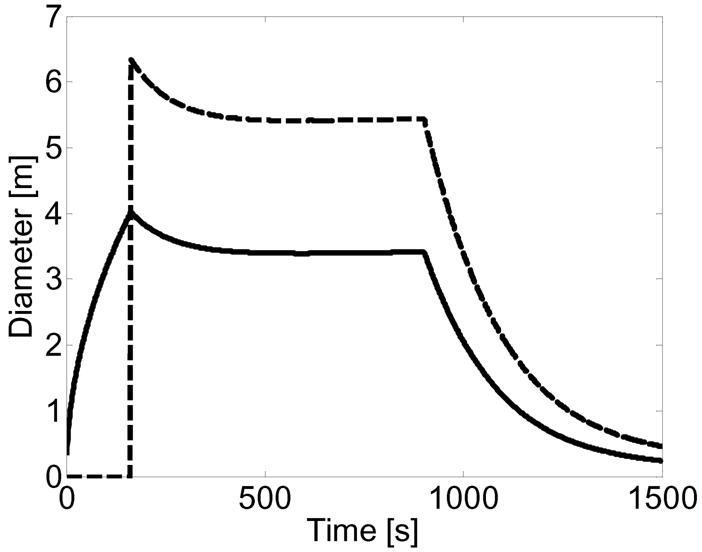

Figure 2: Pool (solid line) and the flame (dashed line) diameters

When the leakage is cut off after 15 minutes, the pool-fire extinguishes rather quickly according to the burning rate of 0.066 kg/m^{2}s (see also Rew and Hulbert, 1996).

Figure 3 shows the temperature of the liquid inside the intermediate vessel and the radiative heat absorbed by that unit. Figure 4 shows the same variables referred to the storage tank. When the outflow is cut off, the intermediate vessel becomes like a batch unit and its temperature increases due to the radiative heat from the fire is not partially removed by the liquid flux. Finally, when the pool-fire extinguishes, the temperature decreases because the heat dispersion to the environment (see Figure 3). Conversely, the temperature of the storage tank has a sluggish dynamics due to the larger holdup (see Figure 4).

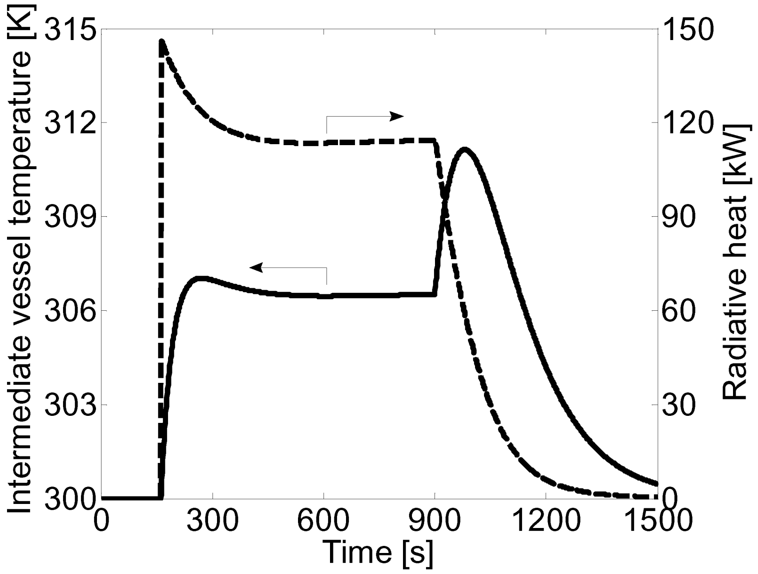

Figure 3: Intermediate vessel temperature (solid line) and absorbed radiative heat (dashed line)

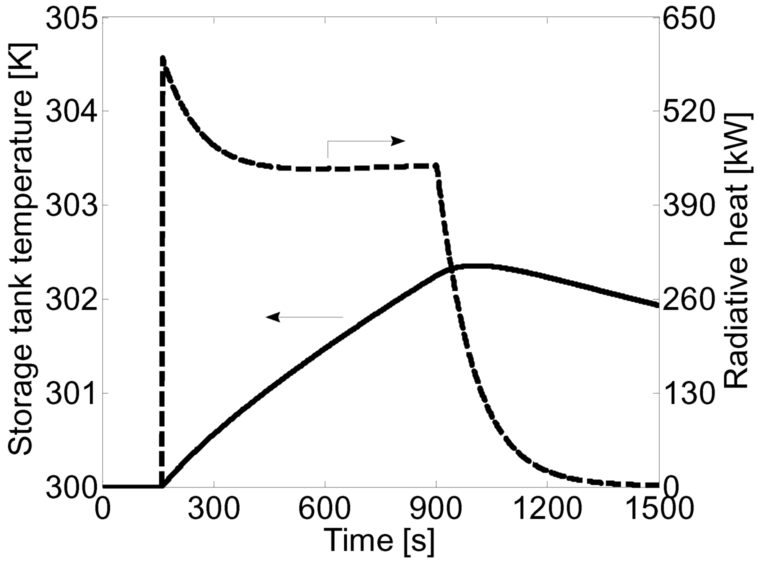

Figure 4: Storage tank temperature (solid line) and absorbed radiative heat (dashed line)

The temperature increases in the storage tank and in the intermediate vessel cause a few secondary effects:

- the liquid volumetric expansion that causes an increase of the liquid level;
- a partial evaporation of the liquid toluene;
- the increase of the pressure according to the gas holdup.

Consider that a temperature increase of 6 K is usually enough to cause a corresponding increase of the vapor pressure of 20 mbar, a value that can cause the collapse of an atmospheric storage vessel (Lees, 2004). In this case, the intermediate vessel experiences a temperature increase of about 15 K that corresponds to a pressure rise of about 44 mbar, *i.e.* twice the typical value for the roof collapse. The storage tank experiences a temperature increase of about 2.5 K with a corresponding pressure rise of about 5.6 mbar.

This analysis shows that the intermediate vessel can suffer major damages if it was not designed to resist to such an overpressure.

6. CONCLUSIONS

The manuscript introduced the concept of dynamic accident simulator and discussed briefly the features that it needs to be titled with the “dynamic” attribute. The dynamic feature is related to the capability of an accident simulator to follow the evolution of an accidental scenario, in particular, when the variations of the source term are concerned. As far as the release of a liquid is concerned, it is necessary to model the following phenomena: the automatic switch of the liquid pool from spreading to shrinking, its vanishing, the release in a bund, the ignition of the vapors, the evaluation of the pool-fire geometry and its view factors. By implementing a model able to account for these features, the accidental event can be better characterized, simulated, and understood. The manuscript showed a different paradigm in the field of the accident simulation for risk assessment, emergency preparedness, and accident investigation. In fact, by coupling a dynamic accident simulator to a dynamic process simulator, it is possible to consider the influence of the actions of both the control system and the operators on the source term and, consequently, on the accident evolution. This link allows also accounting for the feedbacks between the plant and the accident (*i.e.* they may get influenced reciprocally). The possibility to simulate dynamically the biunique interactions between the process and the accidental event allows increasing and enhancing the training features of the OTS program.

Finally, the manuscript showed the implementation of the aforementioned features in a program called AXIM™. The manuscript discussed only the modeling of a liquid release, although the proposed accident simulator can account also for jet streams, gas dispersions (either dense or passive), and vapor cloud explosions.

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