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## Coupling of integral methods and CFD for modeling complex industrial accidents

Andrea Rum, Gabriele Landucci\*, Chiara Galletti

Department of Civil and Industrial Engineering, University of Pisa, Italy

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## ABSTRACT

Safety enhancement of operations in the chemical and petrochemical industry requires for advances in the tools aimed at supporting risk estimation and evaluation. In conventional risk studies, consequence assessment is carried out through simplified tools and conservative assumptions, often resulting in overestimation of accident severity and worst-case scenarios. Computational Fluid Dynamics (CFD) may overcome the limitation of simplified approaches supporting the study of the dynamic evolution of accidental scenarios and, eventually, the consequences analysis of major accidents. However, the complexity of the problem makes the simulations too computationally demanding; hence an interesting approach is to couple simplified tools based on integral models and CFD. This work is aimed at modeling a safety critical scenario, i.e. domino effect triggered by fire. An integral model is adopted to reproduce a large-scale pool fire, thus simulating the radiative heat received by an exposed pressurized vessel. The behavior of the latter is then modeled through CFD, to investigate the heat-up process and the consequent pressure build up. Potential benefits and limitations of coupling distributed and integral models to support consequence assessment studies are discussed.

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## 1. Introduction

Safety enhancement of operations in the chemical and petrochemical industry requires for advances in the tools aimed at supporting risk estimation and evaluation. Risk analysis uses engineering and mathematical techniques (Crowl and Louvar (2011)), to evaluate consequences of accidents and thus their potential impact (Mannan (2012), Center of Chemical Process Safety (2000)). As remarked by several authors (e.g., Kalantarnia et al. (2009), Landucci and Paltrinieri (2016)), in the consolidated procedures for quantitative risk assessment (QRA), conservative simplifications and a rather static approach are adopted for the consequence assessment of fires/explosions (I et al. (2009)) or toxic dispersion and contaminations (Seguí et al. (2014)). This is due to the high number of potential scenarios and uncertainties related to accident identification and characterization. However, neglecting the transient and dynamic effects associated with the complex accident evolution may lead to inaccurate estimation of the risk. Updates and implementation of continuously changing quantities, the

mitigation effect of safety barriers, and eventually knowledge and evidence on hazard dynamic evolution need to be accounted for a more accurate accident scenario simulation and, thus, for the risk estimation (Villa et al. (2016), Xin et al. (2017), Zarei et al. (2017)). Cascading events represent a critical safety issue characterized by a complex dynamic evolution (Khakzad and Reniers (2015)) and may constitute high-consequence chains of accidents (Darbra et al. (2010), Reniers and Cozzani (2013)). In case of a cascading effect, a primary accident, such as a fire occurring in a primary unit, propagates to neighboring units triggering secondary accidents in the surrounding plant area, with potential amplification of consequences (Necci et al. (2015)).

Commonly applied approaches for the safety and risk assessment of this type of scenarios are not yet consolidated and are based on strong simplifications. As reported by Alileche et al. (2015), damage and escalation thresholds are commonly applied to identify secondary scenarios, possibly resulting from a domino effect. The results of consequence analysis models, applied to the simulation of primary scenarios, are compared to the threshold values, identifying a maximum credible escalation radius (Cozzani et al. (2007)) and performing a screening of escalation events (Cozzani et al. (2013)). This type of screening is important to assess the credibility and the criticality of different escalation scenarios,

\* Corresponding author.

E-mail address: [gabriele.landucci@unipi.it](mailto:gabriele.landucci@unipi.it) (G. Landucci).

but the detailed analysis of critical units requires more advanced tools, such as distributed parameters models.

Computational Fluid Dynamics (CFD) modeling is a consolidated tool to support industrial projects development and was recently adopted in the framework of consequence assessment and safety studies (Schmidt (2012), Landucci et al. (2016b)). The advanced features of CFD models make them a promising tool to support the assessment of complex accidental scenarios, such as three-dimensional pool fires, jet fires and the possible induced cascading events. Such features correspond to: handling complex three-dimensional geometries and environments (e.g. Pontiggia et al. (2010, 2011), Derudi et al. (2014)), analyzing turbulent reactive or non-reactive flow of compressible or non-compressible fluids (e.g. Ferziger and Peric (2002), Lomax et al. (2002)) and analyzing multi-phase flows. Hence CFD may be used to simulate the thermal load on a process vessel due to an accidental fire (Masum Jujuly et al. (2015)) and to investigate the transient behavior of the stored fluid and structure (Bi et al. (2011), Jang et al. (2015)) during heat-up.

Several studies were aimed at simulating industrial fires through CFD based tools (Chenthil et al. (2015), Singh et al. (2014)). Pool fire modeling through CFD has been extensively carried out since the 90's, determining the potentialities of distributed parameters codes in capturing the effects of bunds, wind profiles and confinement in the determination of flame structure and associated effects (Sinai and Owens (1995)). More recently, Sun et al. (Sun et al. (2015), Sun and Guo (2013)), provided a dynamic LNG pool fire simulation to estimate mitigation through high expansion foam at different burning times. Several authors proposed pool fire simulations to analyze the potential occurrence of cascading events (e.g., Bainbridge and Keltner (1988), Masum Jujuly et al. (2015), Siddapureddy et al. (2016)). However, they focused on the determination of the thermal loads distribution on the outer surface of the vessels engulfed by the flames (Siddapureddy et al. (2016)) or exposed to distant source radiation (Masum Jujuly et al. (2015)), while the complex behavior of the tank lading was not taken into account.

Due to the high turbulence, jet fire modeling is also a challenging task that was addressed in recent years (Ferreira and Vianna (2016), Hooker et al. (2016), Sun et al. (2017), Zhao and Magenes (2016)). Wang et al. (2014) adopted FireFOAM to study the radiation characteristics of hydrogen and hydrogen/methane jet fires, capturing the fluctuations in flame length and radiant fraction. Jang et al. (Jang et al. (2015)), simulated a hydrogen jet fire from an accidental leak, determining the dynamic evolution of the flame temperature and shape into a complex three-dimensional layout. A real scale pipe rack was reproduced, determining the flame impact zone as well as the heat radiation profiles. The utilization of CFD to support three-dimensional QRA studies is also documented in other studies (e.g., I et al. (2009)).

The analysis of the transient behavior of tanks exposed to either pool or jet fires was developed since the early 70's by the US Federal Railroad Administration and Transport Canada (Johnson (1998b, 1998a)). Since then, several studies were undertaken, focusing on the thermal response of LPG tanks exposed to fire (Moodie (1988)). Lumped-parameter models (Aydemir et al. (1988), Beynon et al. (1988), Birk (1989), Dancer and Sallet (1990), Graves (1973), Heymes et al. (2013), Johnson (1998b, 1998a), Ramskill (1988), Salzano et al. (2003)) represent the simplest modeling approach to the problem, needing limited computational time and set-up parameters but usually neglecting important complicating phenomena such as the liquid thermal stratification and expansion (Landucci et al. (2016a)).

Distributed parameters models were applied to the assessment of similar problems, e.g. to the analysis of the heat-up of water in

pressurized tanks (Gandhi et al. (2013), Han et al. (2009)), of asphalt in cylindrical tanks (Costa et al. (2013)) or cryogenic liquids (Das et al. (2004), Ren et al. (2013), Roh et al. (2013), Wang et al. (2013)) exposed to external heat sources. Some studies were devoted to the analysis of small scale tanks containing pressurized hydrogen gas exposed to localized fires, supported by specific experiments (e.g., Zheng et al. (2012, 2013)). Therefore the experience with CFD tools is limited to the simulation of the dynamic evolution of fluids with physical and chemical features completely different with respect to LPG and, more in general, to pressurized liquefied hydrocarbons. Only recently CFD models were developed to study the effect of fire exposure on LPG tanks. Bi et al. (2011) considered small-scale LPG tanks, whereas Landucci and coworkers (D'Aulisa et al. (2014), Landucci et al. (2016a)) analyzed large-scale LPG vessels. However, the simulation set-up did not allow to model complex fire scenario exposure. In fact, the heat load was derived empirically or from literature, considering only symmetric and homogeneous heat flux conditions. Moreover, the adopted computational discretization only allowed to separately tracing the liquid and vapor phases, imposing the initial filling level and simulating in details the sole evolution of the liquid phase.

Another key issue that may be investigated through distributed parameters code is the structural response of equipment when exposed to fire. In this case, finite elements modeling (FEM) may be applied for the assessment of the mechanical behavior, thus supporting the prediction of failure conditions, as documented in several industrial studies (e.g., Andreev and Harmuth (2003), Feng et al. (2013), Li et al. (2014)). Saldi and Wen (2016) adopted a specific model for the failure assessment of hydrogen cylinders for automotive applications. In the review presented by Godoy (2016), the buckling problems of atmospheric tanks under static or quasi-static loads were investigated and specific modeling approaches were discussed considering accidental fire exposure. The coupled assessment of the thermal and mechanical response was undertaken for light fuel oil storages (Rebec et al. (2016)) and pressurized gas pipelines (Jang et al. (2015)). In this case, FEM and CFD are adopted to reproduce heat flux exposure conditions and to predict the eventual failure conditions. To the best of our knowledge, this was not undertaken in a coupled way for pressurized tanks. In fact, Landucci et al. (Landucci et al. (2009a, 2009b, 2009c)) and Manu et al. (2009) provided detailed examples of the simulation of LPG tanks exposed to fire, in order to estimate the time to failure and to characterize the escalation scenarios. However, in this latter case, the integration of different modeling approaches for the comprehensive characterization of cascading event chains is not yet consolidated.

The present study focuses on the analysis of pressurized vessels exposed to fire. This type of accidental situation may lead to severe cascading events following the catastrophic rupture of vessels. In the case of storage or processing of flammable liquefied gases under pressure, such as propane, butane, propylene, etc., a BLEVE (Boiling Liquid Expanding Vapour Explosion) may occur (Reid (1979), Venart (1999)), eventually followed by fireball (Abbasi and Abbasi (2007), Maillette and Birk (1996)).

A multi-level approach for the advanced simulation of accident scenarios involving cascading events will be proposed. This is based on coupling advanced boundary condition, based on integral modeling, to distributed parameters modeling. In particular, the work aims at improving a previous CFD model of a pressurised tank described in D'Aulisa et al. (2014) and Landucci et al. (2016a) in order to assess its response in case of complex fire exposure conditions. The latter are imposed by simulating the primary fire through integral models available in literature (Mannan (2012), Van Den Bosh and Weterings (2005)) and coupling the results into the CFD model through bespoke subroutines. The potentiality of the

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