



## Effect of Large Obstacles on High Momentum Jets Dispersion

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Dispersion of toxic and flammable materials from Chemical industries represents a major issue in Risk Analysis; presently, integral models are generally used to assess dispersion consequences, due to the low CPU and time requirements connected to the use of these tools.

Nevertheless, they are mainly developed and tuned for releases in open field (open spaces without relevant obstacles), and therefore they cannot properly account for the geometrical features of the dispersion domain. Computational Fluid Dynamic, on the other hand, allows a full 3D analysis, thus accounting for all the obstacles influence on the flow field, but it involves large computational requirements. In case of gas discharge directed towards nearby large obstacles, an impinged jet is expected: if the jet hits a nearby obstacle, the gas velocity suddenly drops, minimizing the inertial dispersion phase, thus reducing the relevant air entrainment and generally increasing the damages distances. Impinged release models are included in some commercial integral models for consequences assessment even if a clear method to decide when to use them is often missing.

The aim of this work is to provide a comparison between the two approaches (CFDs vs. integral tools) in predicting damage thresholds for both impinged and non impinged jets. A realistic case-study of industrial interest was set-up and the fine tuning of all the involved models and parameters (turbulence modeling, geometry description, mesh independence, etc.) was finalized.

### 1. Introduction

Dispersions of toxic and flammable materials from Chemical industries represent a major issue in Risk Analysis, since they usually reach very large damage distances thus potentially involving a great number of people both inside and outside the plant; presently, integral models (simplified, uni-dimensional models) are generally used to assess dispersion consequences, such as DEGADIS, SLAB, ALOHA (BernatikLibisova, 2004) and UDM (Pandya et al., 2012), due to the low CPU and time requirements connected to the use of these tools. Integral models are lumped-parameter models, usually pseudo one-dimensional, which account for some physical phenomena using semi-empirical relationships whose parameters are tuned on field test data (Hanna, 1994). Thus, they are mainly developed and tuned for releases in open field (open spaces without relevant obstacles), and therefore they cannot properly account for the geometrical features of the dispersion domain (Brook et al., 2003). Significant obstacles produce eddies, wakes, stagnation and recirculation points that can enhance or reduce mixing with fresh air, thus strongly influencing damage distances (Calhoun et al., 2000). Computational Fluid Dynamic, on the other hand, consists of the numerical solution of the Navier-Stokes transport equations over a computational domain spatially discretized through the definition of a calculation grid. This approach allows for a full 3D analysis, thus accounting for all the obstacles influence on the flow field as discussed in previous works (Busini et al., 2012, Busini et al., 2011, BusiniRota, 2014, Derudi et al., 2014, Pontiggia et al., 2012, Pontiggia et al., 2010, Pontiggia et al., 2009, Pontiggia et al., 2011), but it involves large

computational requirements (Tauseef et al., 2011, Steffens et al., 2013, AiMak, 2013, TominagaStathopoulos, 2013).

In case of gas discharge directed towards nearby large obstacles, an impinged jet is expected: high momentum jets in open field are characterized by high velocities relative to the ambient air, thus involving a significant air entrainment; if the jet hits a nearby obstacle, the gas velocity suddenly drops, reducing the air entrainment and generally increasing the damages distances.

Impinged release models are included in some commercial integral models for consequences assessment; since the use of the impinged vs. the open field model can produce large differences in damage distance, a reliable criterion to select the most appropriate model based on jet characteristics and release geometry is required.

The aim of this work was to work out a comparison between the two approaches (CFDs vs. integral models) in predicting damage thresholds for both impinged and non-impinged jets with a realistic case-study of industrial interest. Results of the two approaches were compared in order to obtain:

- 1) a cross check of the CFD results in open field (thus validating the effectiveness of the CFD models in predicting the effect of atmospheric turbulence in open field, where the integral model are largely validated);
- 2) a validation of the CFD capacity in describing the interaction between high momentum jets and geometrical obstacles in the near field, verifying that the initial loss of momentum of the impinged jet would resolve in lower initial fresh air entrainment and therefore longed damage distances;
- 3) a comparison between CFD and integral methods predictions of impinged jet damage distances, to verify the over-conservative approach of integral methods;
- 4) a solid and time effective simulation approach to be applied in a massive number of CFD runs to build up a criterion to evaluate the best available model for impinged jet dispersions.

## 2. Materials and Methods

In this work, CFD was used to perform the simulations coupled with the AsSM (Pontiggia et al., 2009) for the description of an atmospheric stability class consistent with Monin-Obhukov similarity theory profiles across the integration domain. Thus fully developed vertical profiles of velocity, temperature, turbulence intensity, and dissipation rate were used as boundary conditions at the wind inlet boundary. Standard boundary conditions were used for all the other boundaries (as reported in Table 1). The commercial package Fluent 12 (ANSYS Inc., 2009) was used for all the computations.

## 3. Results and Discussion

The case-study treated is part of a regasification plant in which an accidental release of methane gas was hypothesized. The jet is coming out of an Open Rack Vaporizer (ORV) and disperses in atmosphere leading to a steady-state release. In the vaporizer the methane is stocked in gas phase at the absolute pressure of 65 bar and at a temperature of 4,5 °C. The hole diameter is 0,0254 m (1 inch) and positioned at the centre of the pipe external surface.

Firstly the open field dispersion of natural gas was modelled for a neutral stability class and 5 m/s wind speed at 10 m above the ground with the suite package PHAST in order to define the dimension of the expanded diameter, the final velocity of the jet (i.e., the velocity of the jet in correspondence of the expanded diameter) and the mass flow rate. The release is sonic and the gas calculated velocity after the atmospheric expansion is about 377 m/s, the expanded diameter is 0.7037 m and the mass flow rate is 5.54 kg/s and the gas temperature is -65.72°C. The CFD simulations were performed considering the estimated condition of the release, the density of the gas was modelled as an ideal gas at constant pressure (thus providing only the dependency of density upon temperature).

The geometry of the case-study comprehend the ORV (16mx8mx8m) and the pipeline (10 m long with a diameter of 0.4 m and 1 m far from the ground) as sketched in Figure 1.

The simulated domain was 300mx50mx50m, thus wide enough to ensure the independencies of the simulations results from the chosen domain; it was meshed with a triangular grid for the faces and a tetrahedral one for the volumes, paying attention at the density of the cells, which must be higher in correspondence of the critical spots (such as the hole and the obstacle); to mesh the open field case, about  $6.5 \cdot 10^5$  cells were used. To verify the independence of the results from the used mesh, the simulations were carried on also with a mesh of about  $140 \cdot 10^5$  cells; the results of the two different configurations were comparable.

*Table 1: Boundary conditions used in all the simulations*

Boundary	Type
Wind Inlet	velocity inlet, velocity profile
Wind Outlet	pressure outlet
Top boundary	velocity inlet, velocity profile
Lateral boundary	velocity inlet, velocity profile
Ground	wall, roughness = 0.05 m
Gas Inlet	Velocity inlet, 377 m/s, -65.72 °C
Walls	wall@300 K, roughness = 0.05 m



*Figure 1: domain top global view*

As jet-impinging obstacle, a cylinder 2 m high and with a diameter of 1.5 m was added in the domain and located 6 m far from the hole, as sketched in Figure 1. Obstacle dimensions and location were selected according to typical layout of real regasification plant.

Simulations results are sketched in Figure 2, Figure 3 and Figure 4 in which the the LFL footprints under open field conditions, the LFL footprints in presence of the obstacle and the parity plot of downwind distance reached by the LFL with and without the obstacle (i.e., in case of impingement and free jet) are reported. This allows for an easy comparison between Fluent and PHAST results.

We can see that in open field conditions the CFD results are in very good agreement with the PHAST case, thus validating the effectiveness of the CFD in predicting the effect of atmospheric turbulence in open field. However, the agreement worsens for the impinged jet, therefore confirming the tendency of the methodologies embedded in integral models to overestimate the hazardous distance.

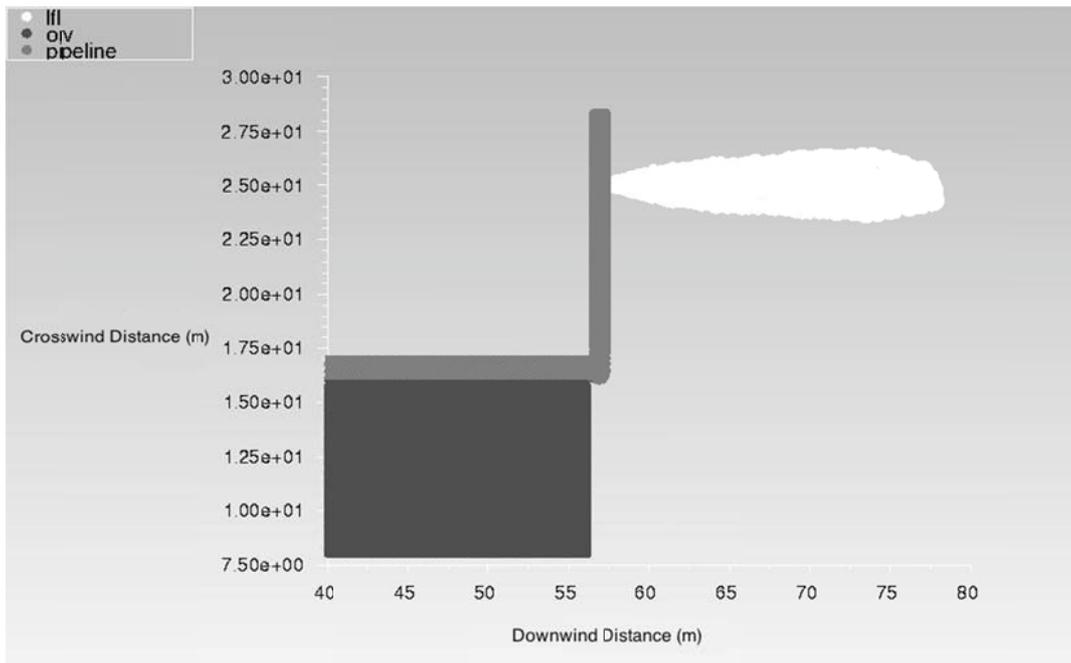


Figure 2: LFL footprint of methane jet under open field condition predicted by the CFD

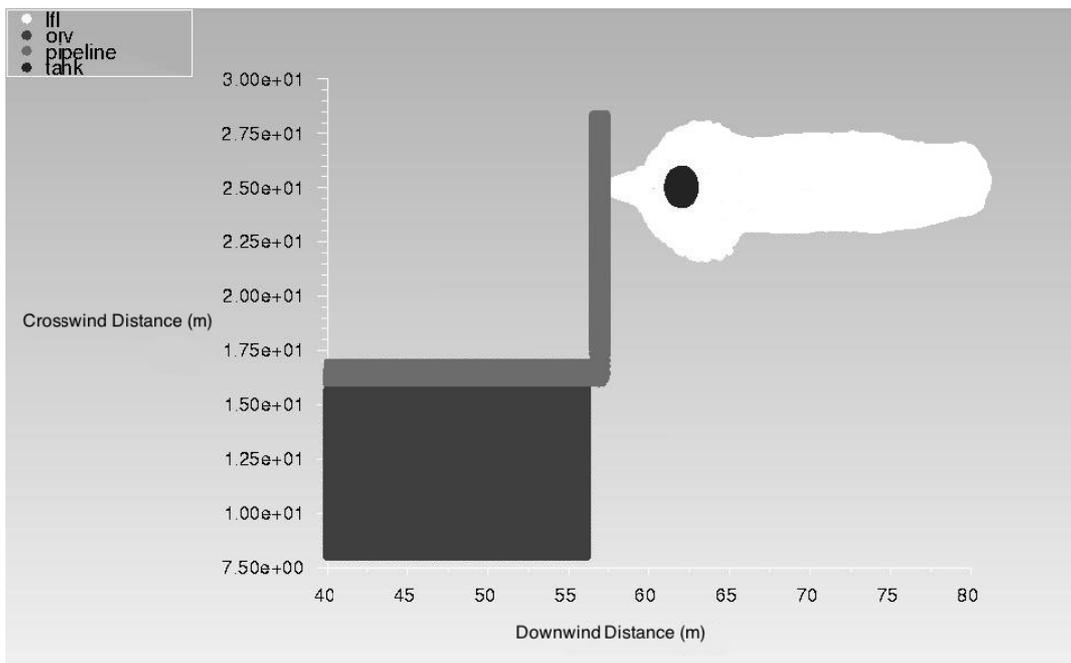


Figure 3: LFL footprint of methane jet under impinging condition predicted by the CFD

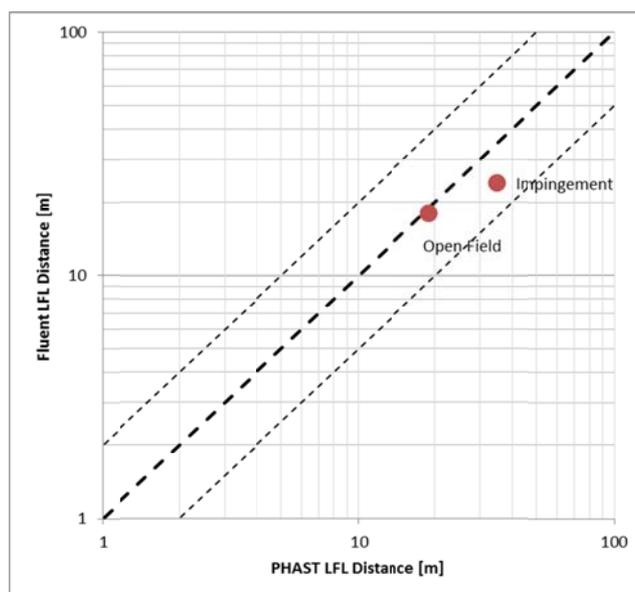


Figure 4 Parity plot of downwind distance reached by the LFL with and without the obstacle

#### 4. Conclusions

This work is focused on the modeling of impinged jet dispersion in the environment: toxic and flammable dispersions are often the most critical events in terms of consequences distances in risk assessment studies, and their potential outcomes can become even worse due to the impingement phenomenon: if the jet hits a large obstacle in the near field (where the gas momentum is still high), the axial velocity is significantly limited, thus reducing the relative velocity with the atmospheric air, and, therefore air entrainment in the initial high momentum dispersion phase.

Integral methods are generally provided with specific models for jet impingement representation: nevertheless, relevant results can be over-conservative; to obtain credible consequences assessment and avoid extreme over-conservative results, it is important to distinguish in a proper way which obstacles can produce jet-impingement and which obstacles are too small or too distant to trigger this phenomenon.

In order to analyze this problem, CFD tools were applied to a realistic case of flammable gas dispersion. The aim of the work was fourfold:

- 1) To validate CFD approach (source term representation, geometry discretization, atmospheric turbulence modeling) for gas dispersion from high momentum jet; this validation was accomplished by means of a comparison among CFD and integral model results under open field conditions: since integral model parameters are tuned on experimental data of open field releases, relevant performances are well established in absence of significant geometrical obstacles. Results (expressed in terms of distance to flammability limits) shown a good capability of CFD in simulating high momentum jet gas dispersion in open field.
- 2) To investigate the physical phenomena involved in the jet impingement scenario: CFDs, being able to predict effects of geometrical features on the flow field, are fully capable to account for obstacle influence in terms of turbulence increasing due to the formation of eddies, wakes and recirculation point. On the other hand, performed simulations, highlighted also the capability of CFDs in correlating the initial velocity loss due to nearby obstacles impingement with the limited air entraining in the high momentum gas dispersion and therefore providing higher damage distances in terms of distance to hazardous gas concentration.
- 3) To compare impinged gas distances forecast by CFDs and integral model: the analysis described in this work has confirmed the general tendency of integral model in overestimating damage distances for impinged jet. This feature raises the necessity for improved correlations between geometric arrangement (i.e. distance between jet and obstacle, dimension of the obstacle, etc.) and the most suitable model to be used in consequences calculation (impinged vs. non impingement).
- 4) To establish a robust and time/resources effective approach for high velocity impinged jet simulation with CFD codes: such an approach will be adopted, as a future work, in order to work

out a massive number of simulation to investigate an empiric relation between scenario description and most suitable modeling approach.

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