# ATMOSPHERIC DISPERSION OF XYLENE EVAPORATING FROM A DRIFTING SLICK

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#### INTRODUCTION

The French research project Galerne deals with marine accidents which involve containers transporting hazardous evaporating chemical substances. The main objective of the project is the writing of intervention instructions for emergency units depending on various accidental scenarios.

Within this project, Meteo-France is in charge of evaluating the transport of the spill of pollution at the sea surface and the atmospheric dispersion of the chemical substance linked to its evaporation. A modelling system has been settled, which consists of the coupling of two models :

- The first one, MOTHY, is Meteo-France operational drift forecast system in case of marine pollution. It is a trajectory pollutant model coupled with an hydrodynamic ocean model.
- The second one, PERLE, is a meso-scale atmospheric dispersion modelling system used in operations in case of accidental releases of pollutant into the atmosphere. Meso-scale meteorological fields are simulated by the nonhydrostatic MESO-NH model (8km and 2km resolution nested grids); a lagrangian particle model, LPDM (M.Uliasz,1994) from the Colorado State University, is used in this study to simulate the atmospheric transport of the pollutant.

The coupling essentially consists in evaluating the moving surface source term for PERLE associated with the simulated drift forecasted by MOTHY and with the evaporation rate using the results obtained by other partners within the project working on the evaluation of evaporation rates depending on the considered pollutant.

Based on various accidental scenarios specified within the Galerne project, different simulations have been performed in order to evaluate the potential impact in terms of atmospheric concentration related to critical thresholds. The simulations consider various meteorological conditions to assess the impact in more or less favourable conditions for evaporation and dispersion in the atmosphere.

# **ACCIDENTAL SCENARIOS**

The first activity within GALERNE project consisted in defining typical accidental scenarios based on a study of marine accident that occurred in the past. This work was conducted by other partners of the project (Bureau Veritas, Gaz de France, BEA Mer, Marine Nationale, INERIS, CEDRE).

Since our activity focused on the evaluation of the atmospheric dispersion of pollutant associated to a slick drifting at sea surface, only scenarios involving non-boiling evaporating species were considered so that the living time of the evaporating pool would be more than a few minutes.

The two accidental scenarios selected for this study consider a release of 2500 ton of xylene into the sea. The first one is fast (15 minutes) with a hole of 1 m<sup>2</sup> on the boat's hull and the second one continuous (24 hours) with a hole of approximately 10 cm<sup>2</sup>.

#### COUPLING OF MOTHY AND PERLE MODEL SYSTEMS

In its operational configuration for accidental release, PERLE deals with fixed source term in space and time. The technical issue within this coupling consist in providing PERLE with a moving surface source term generated by the drifting slick of pollutant simulated by MOTHY associated to a given evaporation rate.

# **Evaporation rate**

The evaporation rate depends on the nature of the pollutant and on environmental conditions such as sea temperature, wind strength at sea surface... Measurement campaigns have been settled within the project in order to evaluate the evaporation behaviour of different species given different external conditions. These activities are ongoing and conducted by other partners of the project (INERIS, CEDRE, Gaz de France). Results of these experiments should be implemented within MOTHY's evaporation module. In our study, the evaporation rate of the Xylene is calculated using a formulation (equation 1) given by Mackay and Matsugu (1973) that is adapted for non-boiling liquid pools for which the evaporation depends mainly on the rate at which the vapour can be removed by the wind above the pool. The evaporation rate is expressed as followed:

$$Q = 0.00487 * (M * P) / (R * T) * V^{0.78} * X^{-0.11} * (v/D)^{-0.67}$$
(1)

where Q is the evaporation rate (g/m2s), M the molecular mass of xylene (106 g/mol), P the vapour pressure (Pa), R the international gaz constant (J/(K.mol)), T the pool temperature (°K), V the wind speed at 10m height (m/s), X the pool diameter (m), v the kinematic viscosity vapour and D the diffusion coefficient of Xylene vapour in air (m2/s).

# Source term reconstitution for atmospheric dispersion

Since MOTHY is a trajectory transport model, the pollution is discriminated into a large number of fictive particle (of different size for vertical motion) which are moving independently from one another. In order to evaluate the evaporated pollutant mass at each time step, the idea is to represent the drifting slick as a surface formed by a number of "elementary" mesh containing at least one particle (figure 1, left picture). Each elementary mesh is responsible for part of the mass evaporated into the atmosphere depending on the mass contained into the mesh (number of fictive particle), the surface of the mesh and the evaporation rate used. Thus, each elementary mesh constitutes an independent source term for PERLE.

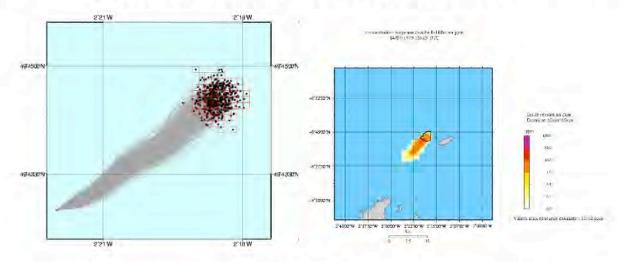


Figure 1.

Left picture: in black, particles representing the pollution slick drifting at the sea surface, in red, associated mesh grid for source term reconstitution; Right picture: example of a plume (color shaded concentrations ppm) resulting from the evaporation of the pool (delimited in black)

The number and the size of elementary mesh is chosen as a compromise between a good representation of the slick shape and a limited number of source terms to be treated by PERLE.

As the pollutant is evaporating, the mass of each particle transported at sea surface by MOTHY is decreasing. When reaching a mass of zero, the particle is re-injected within one of the mesh (with mass transfer from other particles contained in the mesh to the new one) in order to keep a sufficient number of particles to have a realistic representation of the drifting pollution.

# SENSIBILITY TESTS WITH VARIOUS METEOROLOGICAL CONDITIONS

The aim of this study is to test the sensibility of the pollution transport (dispersion of the slick at sea surface and of the evaporated cloud in the atmosphere) to different meteorological situations. Therefore, the two accidental scenarios have been simulated on different dates providing various conditions in terms of stability of the Planetary Boundary Layer (PBL), wind speed near sea level, sea surface temperature, tide coefficient... Six dates have been extracted from Meteo-France B95 data base which provides a classification of typical synoptic meteorological situations for western Europe. The location chosen for the simulation is situated on the Manche sea (Casquets: 49°N 43' -2°N 22').

Table 1. Meteorological conditions for selected dates. Wind speed and sea surface temperature are averaged on simulation period

Date	Wind speed (m/s)	Sea surface temperature	Tide Coefficient	Atmospheric stability	
	(11//3)	(K)	Occincient	(Pasquill)	
24-04-1979	9.4	282.9	95	D	
18-10-1980	7.9	287.5	37	С	
04-07-1979	1.7	288.1	42	F	
07-10-1985	3.9	288.4	89	В	
16-04-1984	3.6	282.6	112	С	
23-04-1991	3.6	282.6	50	D	

Over sea surface, the stability depends mainly !the difference between the sea surface temperature and the air temperature. In western Europe, stable conditions occur generally during summer period when the sea temperature tends to cool the air in contact with the surface. On the contrary, in winter, it warms up the air in contact and tends to unstabilize the PBL. Generally, stable conditions are associated with weak winds (< 5m/s) whereas unstable conditions are associated to more perturbed situations with moderate to strong winds. The first type of situation (stable and weak winds) is well represented on the 4<sup>th</sup> of july 1979 (date 1) whereas the second one (perturbed with stronger winds) is covered by the 24<sup>th</sup> of April 1979 (date 2). Other dates propose intermediate conditions.

The results of simulations have been analysed in terms of evaporation rate, time taken by the xylene to completely evaporate (persistence of the pool), the surface covered by the pool, the maximum distance reached during its drift between the pollution slick and the accident location and finally the air concentration levels reached. These characteristics, summarized in table 2, could be relevant for anticipating the transport scenario in terms of potential impact on emergency units or nearby populations in case of a real accident.

Table 2. Results of simulations for selected dates (short and continuous release). Evaporation, mass transfer and pool surface are averaged on simulation period. For continuous release, the evaporation time is not relevant therefore not mentioned.

Date	Evaporat ion rate (g/(m².s))	Total mass transfer rate (kg/s)	Pool surface (km²)	Total evaporati on time (min)	Max distance of the pool from release	Max air concentr ation reached (ppm)	Release duration
					point (km)		
24-04-	0.79	576	0.7	80	1.9	34.7	15min
1979	0.71	364	0.5		7.7	30.6	24h
18-10-	0.72	775	1.1	60	2.8	25.2	15min
1980	0.62	297	0.5		5.6	26.2	24h
04-07-	0.21	350	1.8	125	8.4	81.9	15min
1979	0.18	169	0.9		6.2	69.5	24h
07-10-	0.33	557	1.6	80	8.6	34.0	15min
1985	0.33	293	0.9		6.6	38.4	24h
16-04-	0.51	666	1.4	60	6.5	33.5	15min
1984	0.33	249	1.0		7.2	22.0	24h
23-04-	0.45	675	1.4	75	5.7	40.4	15min
1991	0.34	241	0.7		5.8	37.3	24h

The results confirm the predominant role of the wind speed in the evaporation rate (0.21 for date 1 against 0.79 for date 2). The persistence of the xylene pool results from the evaporation rate on the one hand and from the pool surface on the other hand. We observe in table 2 that the surface covered by the pool decreases with the wind. Therefore, the influence of the evaporation rate on the total evaporation time of the pool is partially balanced by the influence of the pool surface. This can explain the relatively small differences (persistence between one and two hours) despite contrasted meteorological conditions.

In all conditions and both release scenarios, the distance between the pool and the release location remains below 10 km and the maximum concentration reached is 82 ppm which remains below the toxic threshold for Xylene and is usually located within few kilometers from the pool. Once again, we can observe that differences in concentration levels from one situation to an other are quite small. Stable conditions tend to reduce the vertical dispersion of the pollutant in the atmosphere which tends to increase the concentration. This is balanced by the fact that weak winds (usually associated to stable conditions) tend to reduce the evaporation rate which results in weaker concentrations.

## CONCLUSION

A system composed of MOTHY (drift forecast of marine pollution) and PERLE (atmospheric dispersion) has been setup in order to evaluate the potential impact of an accidental release of xylene into the sea given contrasted meteorological conditions. Two release scenarios have been simulated using real time

meteorological data extracted from past situations. Results of the simulations have shown a small sensitivity of the potential impact in terms of persistence of the liquid pollutant pool, distance covered by the drifting pool, air concentrations reached. These are explained by compensating influences between the evaporation rate and the meteorological conditions.

No matter the environmental conditions, the studied accidental scenarios would lead to limited impact on emergency units or nearby population since concentration levels should stay below critical thresholds and the xylene pool evaporate within one or two hours. Nevertheless, it should be mentioned that provided air concentrations are averaged over 1km² which means that concentrations could locally reach higher levels. We must also keep in mind that the system was tested on only six dates which is a quite small sample of situations even though they have been chosen to represent contrasted conditions. In the future, it will be interesting to re-simulate these scenarios integrating the results of the ongoing experiments on evaporation rate evaluation and to simulate other dates to refine the first conclusions from this study.

The results of these simulations will help to prepare recommendations for emergency units approaching the accidental site and also to give indications of the potential exposure of nearby populations depending of their distance to the drifting pollution slick. In case of a real accident, the system could be activated quite easily integrating real time accidental scenario information and meteorological data.

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