Cedre Information Day

Modelling chemical dispersion

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Plan

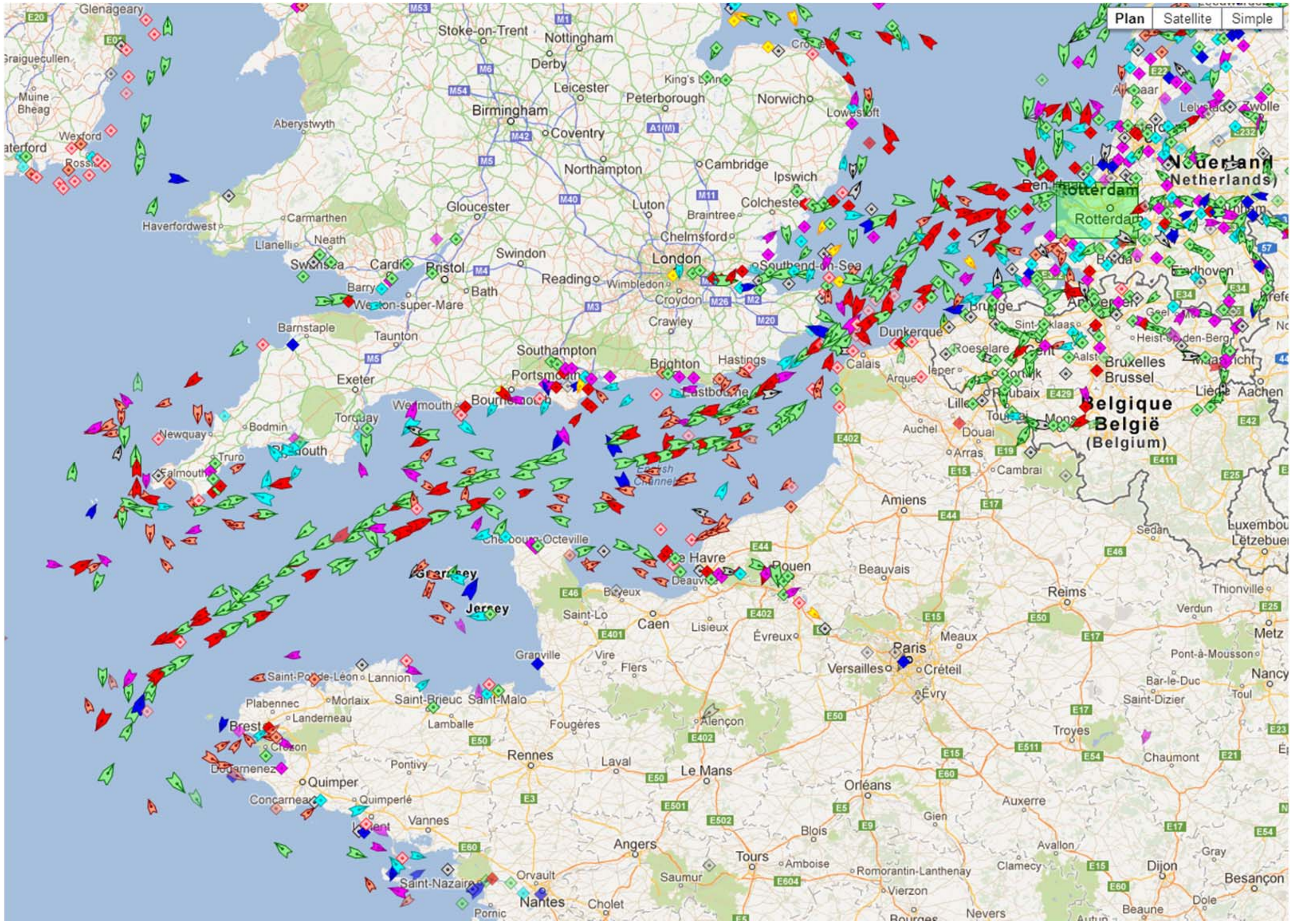
1. **Introduction**
   - *Context*
   - *Phenomenological description*

2. **Dispersion mechanisms in the aquatic environment**

3. **Modelling strategies**
   - *Surface release*
   - *Subsurface release*

4. **Example of modelling**

Context



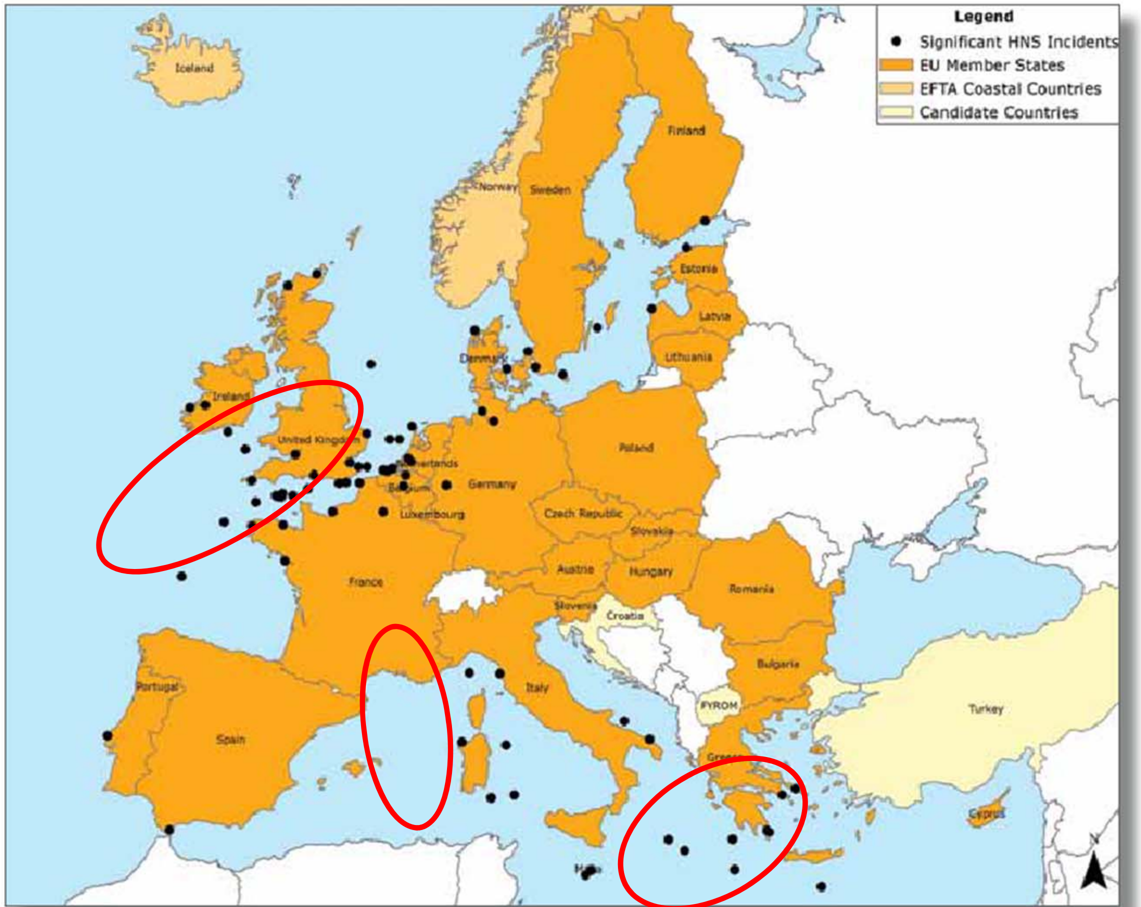
- Passenger Vessels
- Cargo Vessels
- Tankers
- High Speed Craft
- Tug, Pilot, etc
- Yachts & Others
- Fishing
- Navigation Aids
- Unspecified Ships
- Ships Underway

MarineTraffic.com

Context

Significant shipping incidents involving Hazardous and Noxious Substances (HNS)

SIGNIFICANT HNS INCIDENTS (1978-2010)



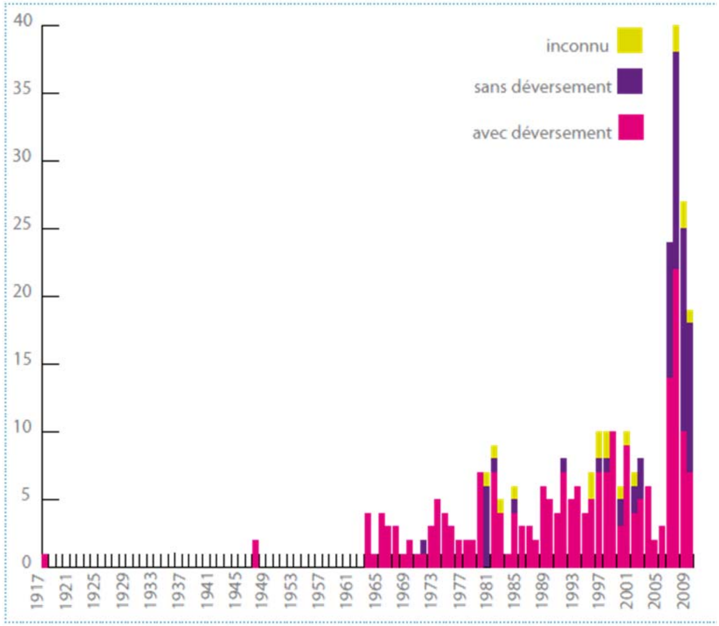
Source: **E**uropean **M**aritime **S**afety **A**gency (**EMSA**)

Context

Evolution of shipping incidents involving HNS

- ► Constant rise in chemical transport by sea

  - ► 3.5-fold rise in chemical shipping in 20 years
  - ► Wide variety of chemicals
  - ► Different physical and chemical behaviour in the marine environment → SEBC code



Number of accidents involving HNS

Increase in the probability of incidents with severe consequences

Context

Wide variety of chemicals transported

Different response strategies

Pollutant characteristics

- Oils
- Chemicals
- Food products

Characteristics of polluted areas

- Sea, ocean, estuaries...
- Marine reserves, protected areas
- Aquaculture, fishing or tourism areas

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Example of an incident

Ievoli Sun (2000)

- **Quantities transported**
  - Styrene: 4000 T
  - Methyl Ethyl Ketone (MEK): 1000 T
  - Iso Propyl Alcohol (IPA): 1000 T

- **Quantities released:**
  - Styrene: 400 T
  - Methyl Ethyl Ketone: 100 T
  - Iso Propyl Alcohol: 1000 T

Leak in the bow thruster compartment

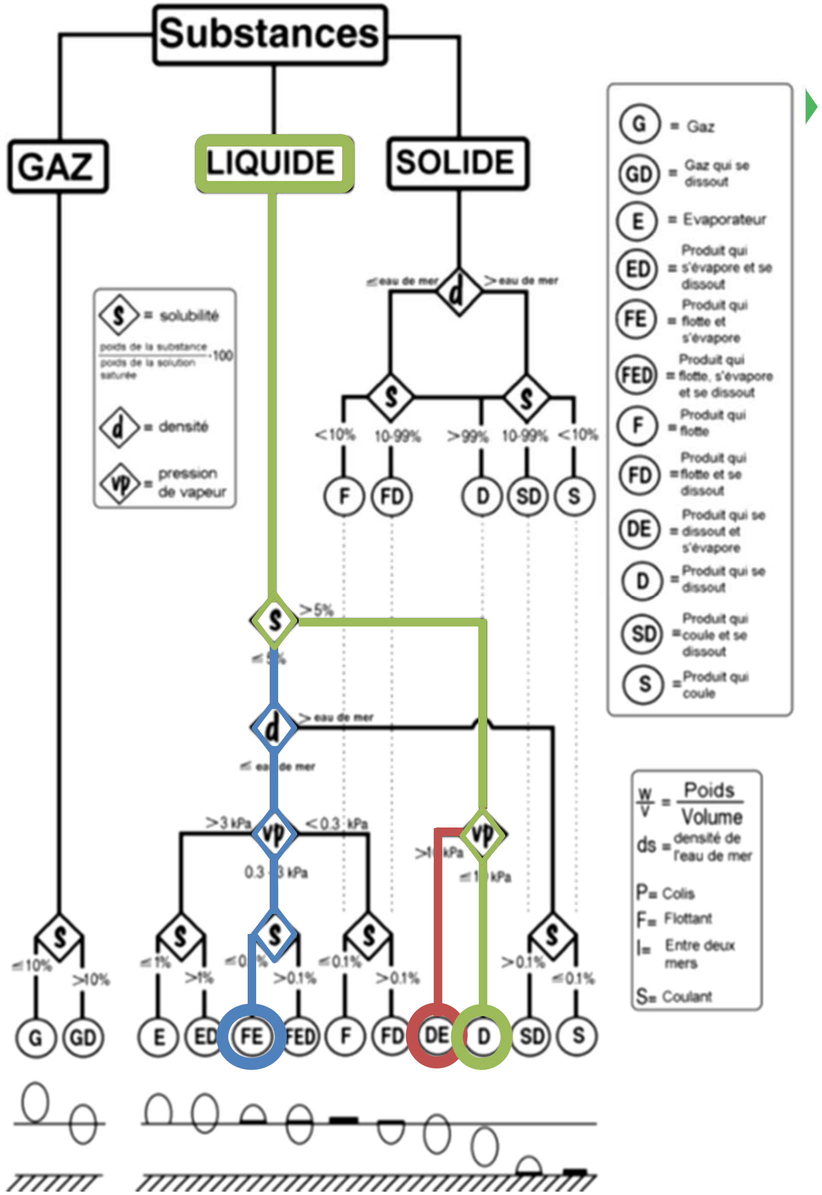
Context

Example of an incident

Ievoli Sun (2000)

	Phase	S [%]	d [kg/m³]	Vp [kPa]	
• Styrene	L	0.03	906	0.667	FE
• MEK	L	26.3	805	10.33	DE
• IPA	L	79	786	4.1	D

- ▶ Formation of a toxic cloud?
- ▶ Risk of fire or explosion?



Phenomenological description

Classification conditions

- Pure substance
- Small quantity
- 20°C
- Atmospheric pressure
- Fresh water

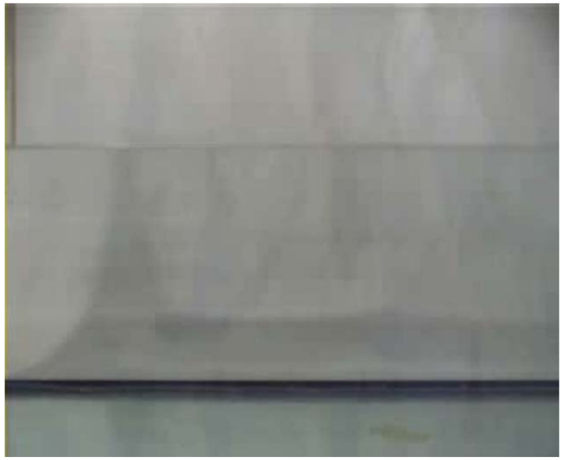
Real conditions

- Not necessarily pure
- Several tonnes
- 4°C
- 10 bars
- Seawater

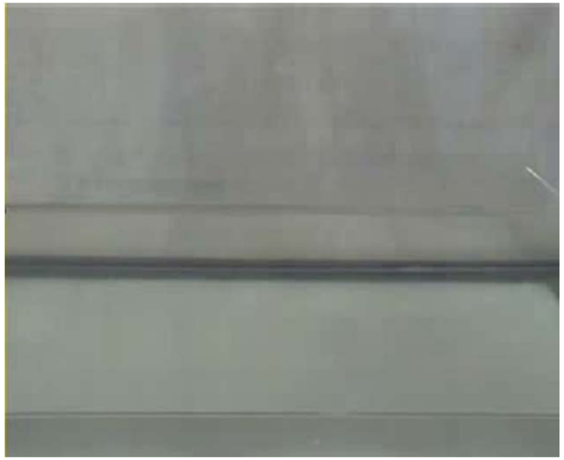
Limitations

- Non-representative conditions
- Possible presence of different products
  - Alteration of dissolution
  - Chemical reaction
- No consideration of dynamics
  - Dissolution
  - Competition between phenomena

Example of behaviours



Sinker (e.g. Toluene Diisocyanate)



Evaporator (e.g. Styrene)

Floater (e.g. Dodecylbenzene)

Dissolver (e.g. butanol)

Dispersion mechanisms

Surface release

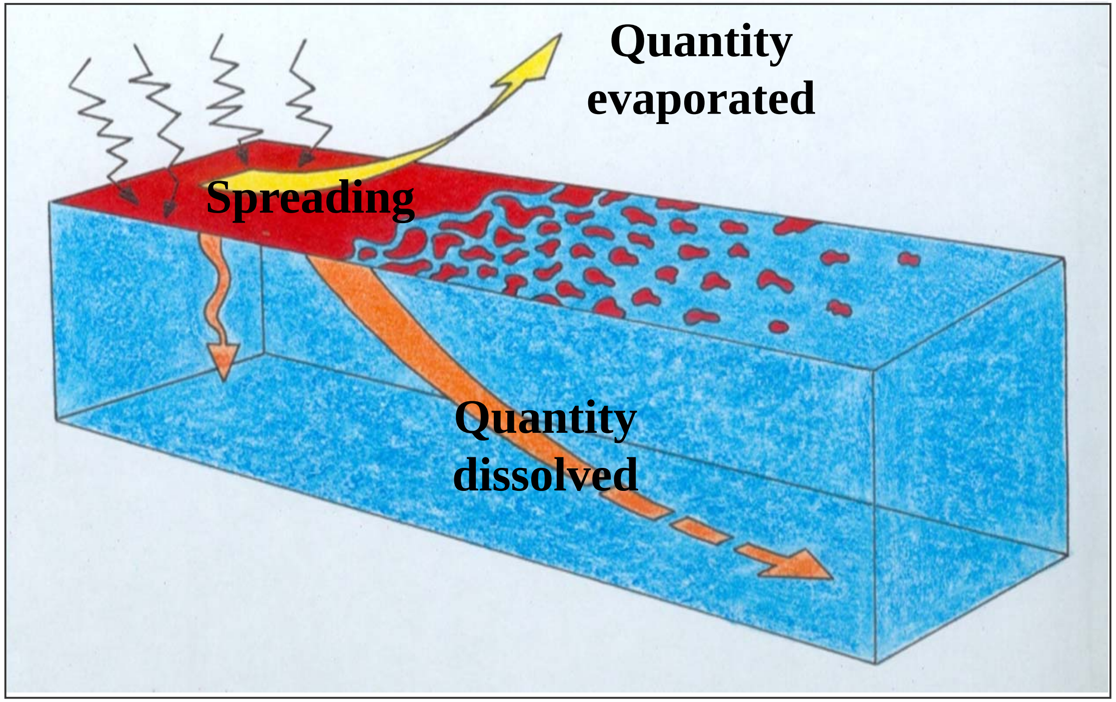
1. Determination of source term (quantity released or rate)-> Bernoulli
2. Material balance according to time

Surface area of the product?

Quantity evaporated?

Quantity dissolved?

How long?



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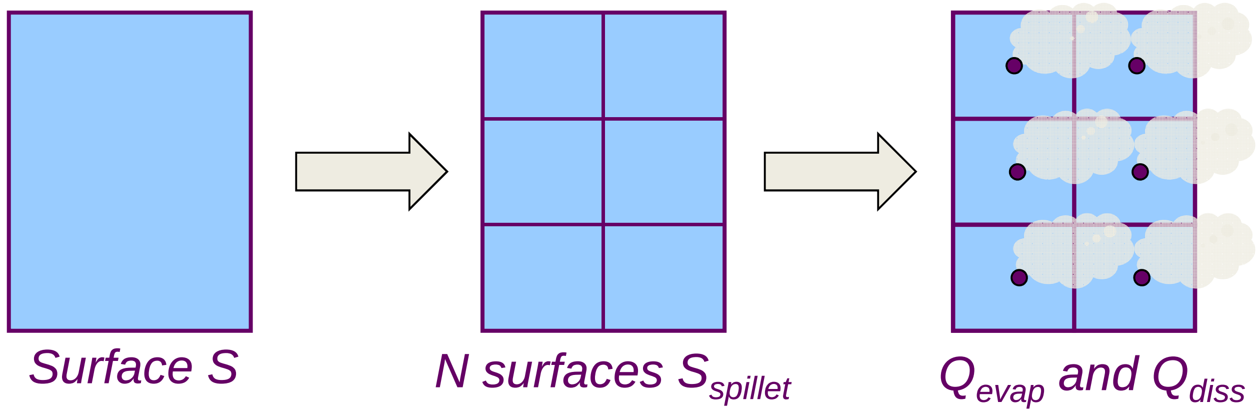
Modelling

Division of slick into unitary elements (spillets) to represent the total surface area of the slick

1. **Calculation of the evolution of each spillet over time (Runge-Kutta discretization scheme)**
   - **Spreading rate of each spillet (*Nihoul, 1983*)**
   - **Quantity evaporated (*Mackay and Matsugu, 1973*)**
   - **Quantity dissolved (*Hayduk and Laudie, 1974*)**

2. **Material balance for each spillet**



Modelling

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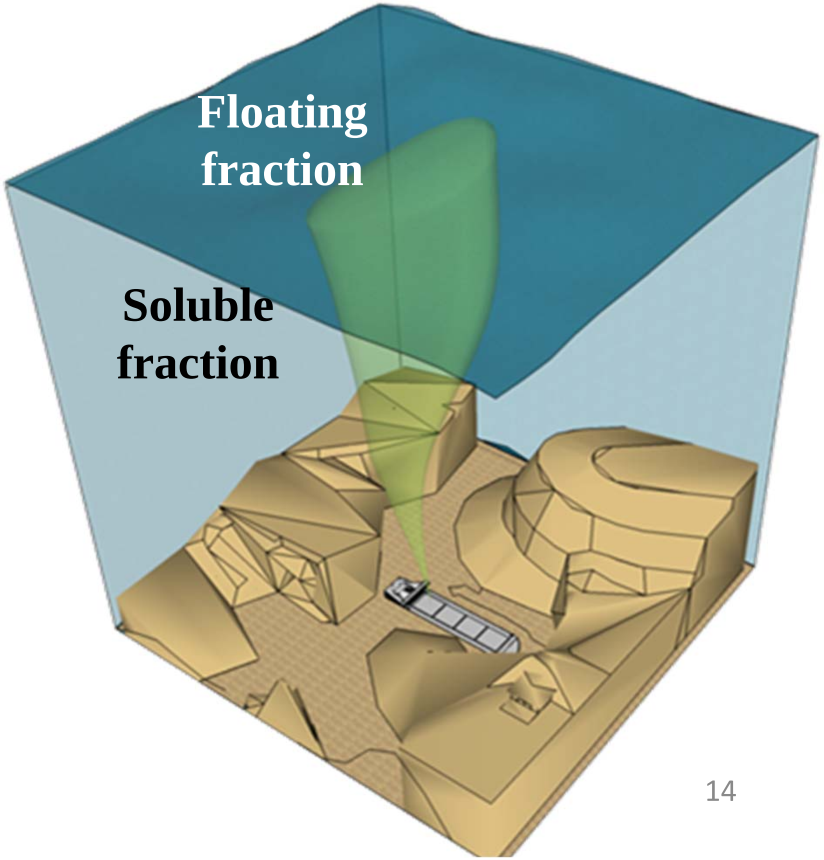
   - Quantity dissolved (*Hayduk and Laudie, 1974*)

2. Material balance for each spillet

3. Coupling with hydrodynamic predictions
   1. Movement of spillets at each time step

Subsurface release

1. Determination of source (quantity released or rate)-> Bernoulli
2. Product dispersion mechanism
3. Upwelling hydrodynamics (speed)
4. Material transfer (dissolution)

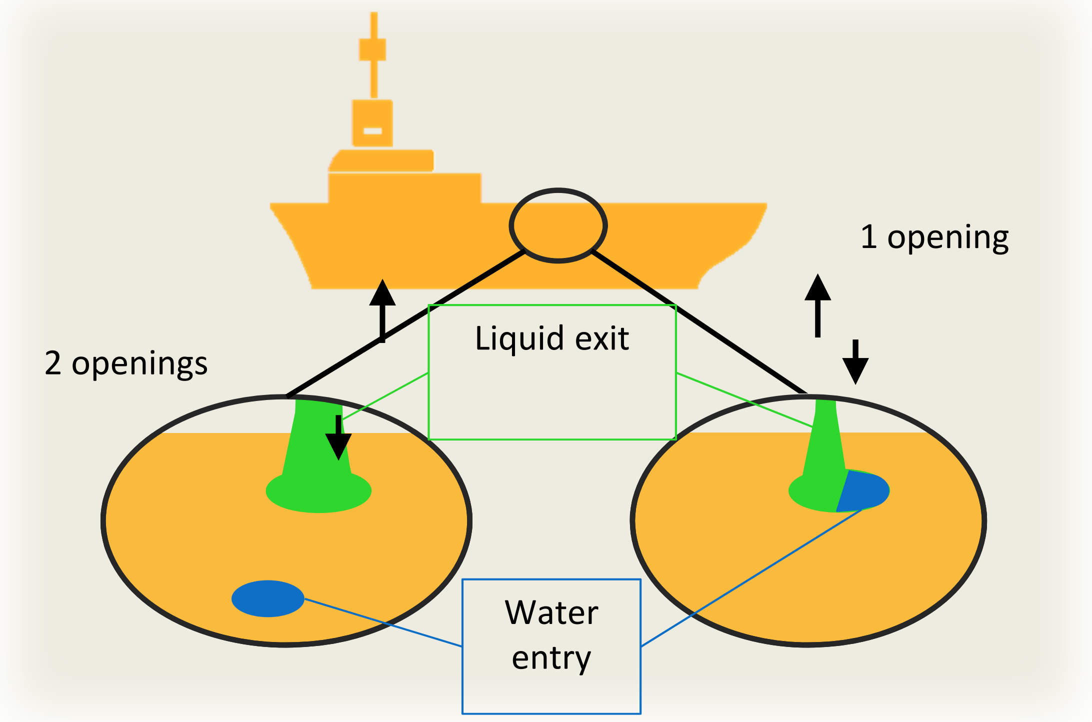


Appearance of substance at surface

- Volume at the surface?
- When?
- How long?

Modelling release rate at breach

1. **Two hydrodynamic behaviours**



2. **Modelling by a local energy balance (Bernoulli)**

Modelling

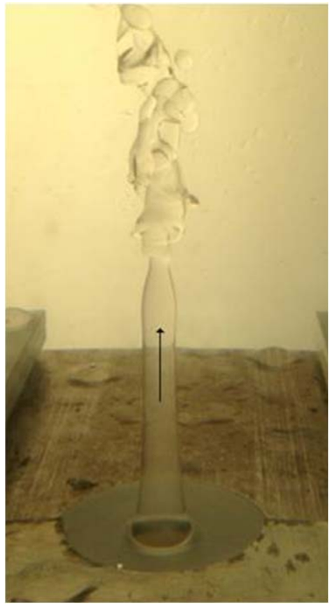
Modelling release rate at breach

Constant rate Q,
Linear section Σ

Diphasic release at the exit opening

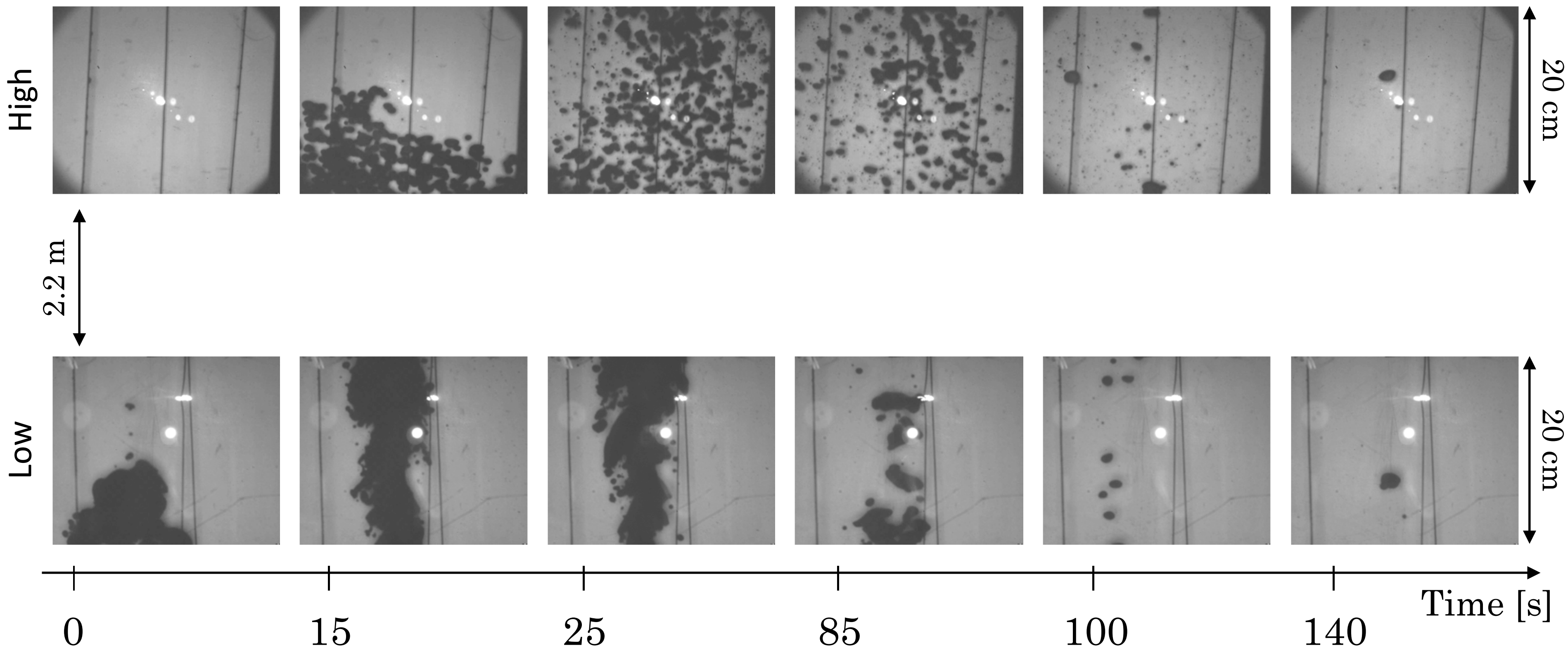
Linear rate Q,
Constant section Σ

Monophasic release at the exit opening



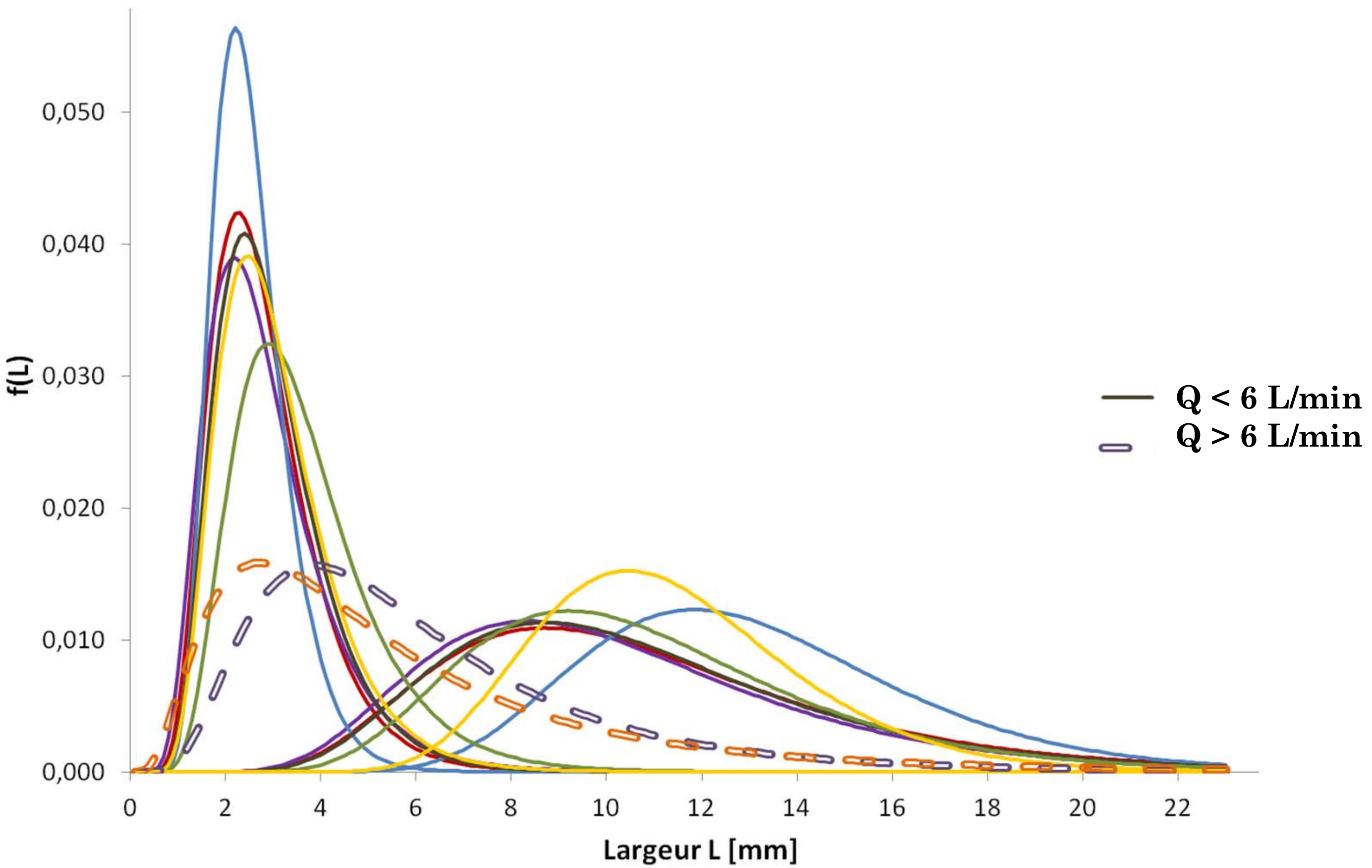
Modelling fragmentation of the leak

Assessment of particle size distribution



Modelling fragmentation of the leak

- 2 types of particle size distributions
- Maximum droplet diameter 22 mm



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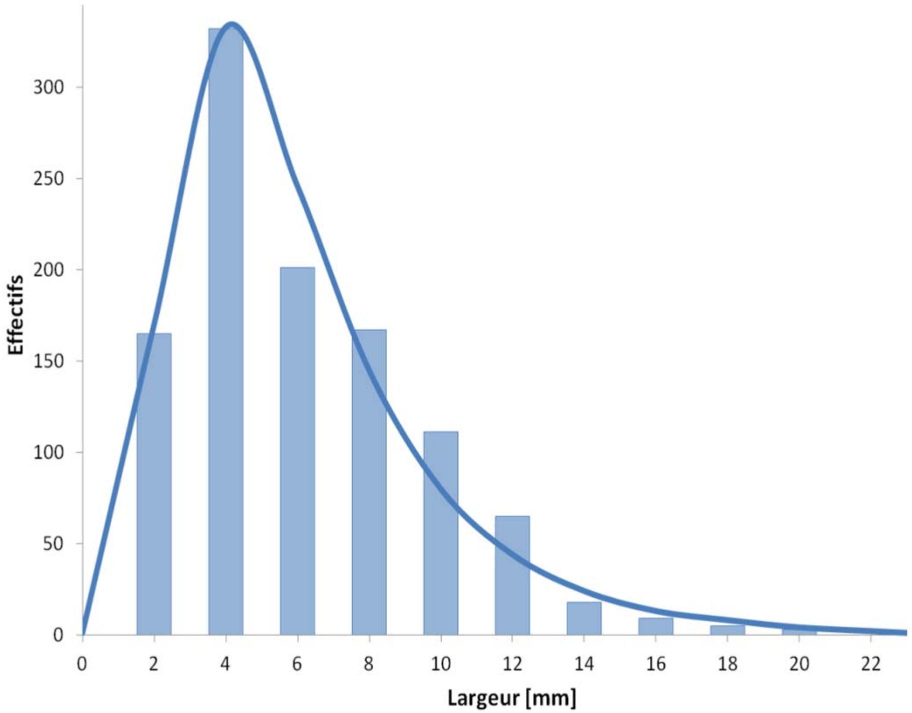
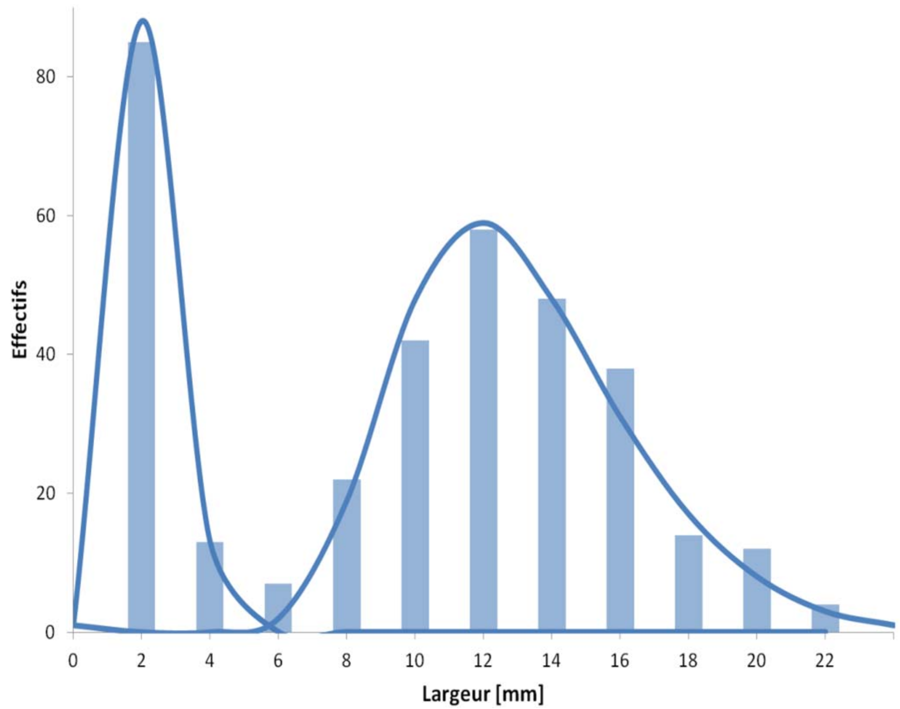
Modelling

Modelling fragmentation of the leak

- Representation of particle size distributions by log-normal
  1. Monophasic release: monomodal distribution
  2. Diphasic release: bimodal distribution



Monophasic release



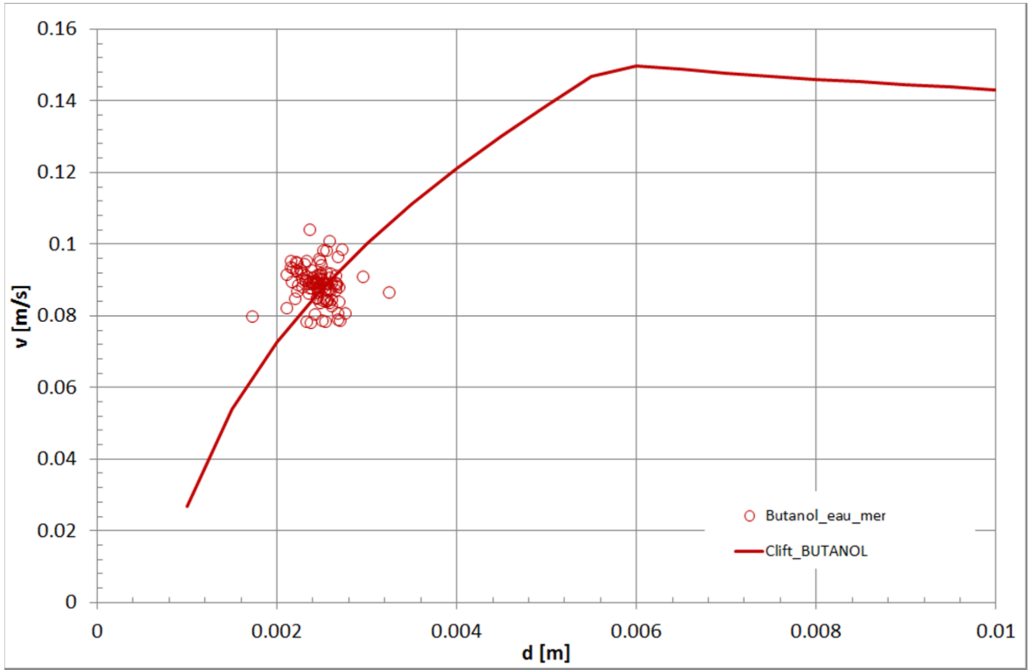
Diphasic release

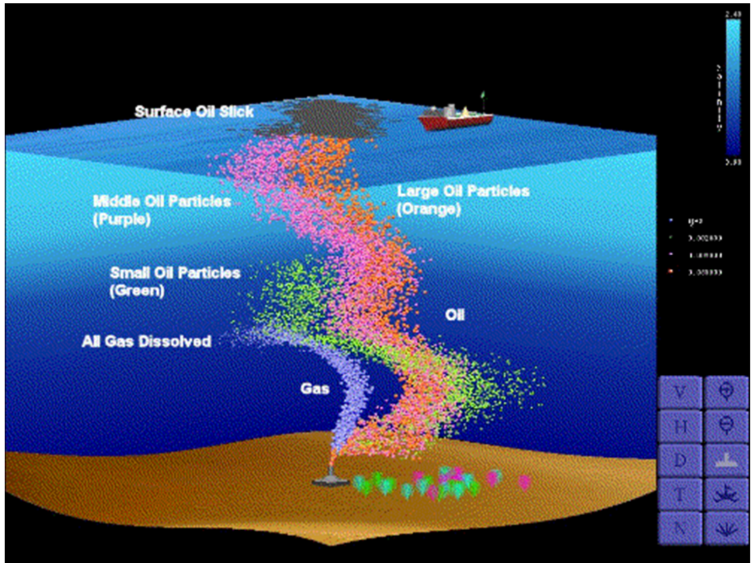
Modelling

Modelling droplet hydrodynamics

1. **Modelling droplet upwelling speed with the Clift correlation (1978)**

2. **Coupling with hydrodynamic predictions to take into account the movement of the bubble plume**



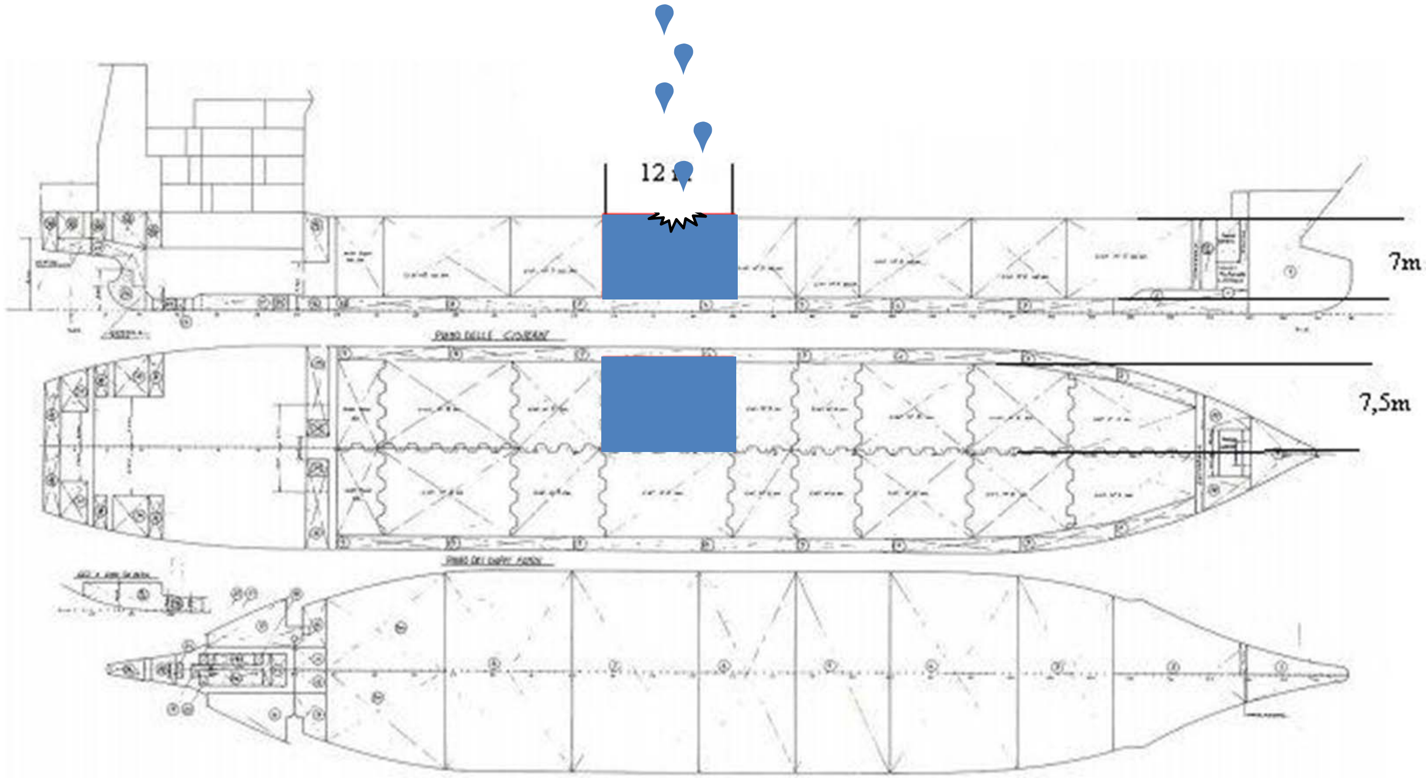


CDOG model, Clarkson Univeristy

Example

Modelling a leak of butanol from a chemical tanker

1. **Leak from a 600 m3 tank**
2. **Breach punctured along 10 cm in diameter**

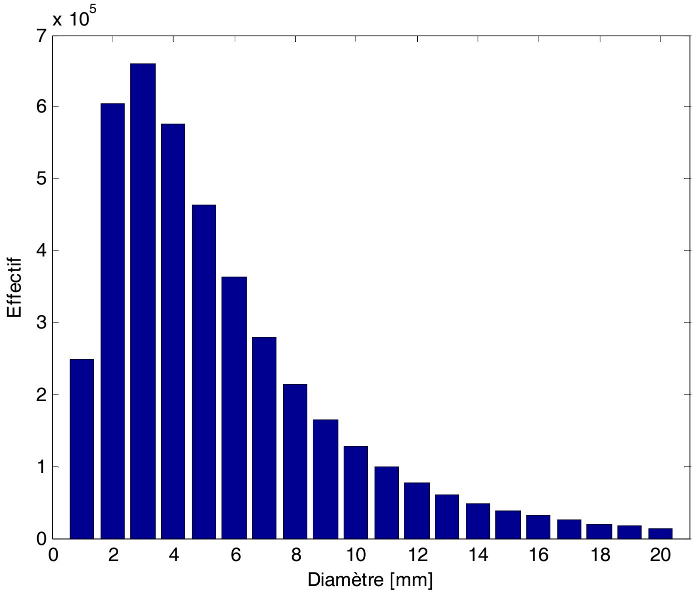


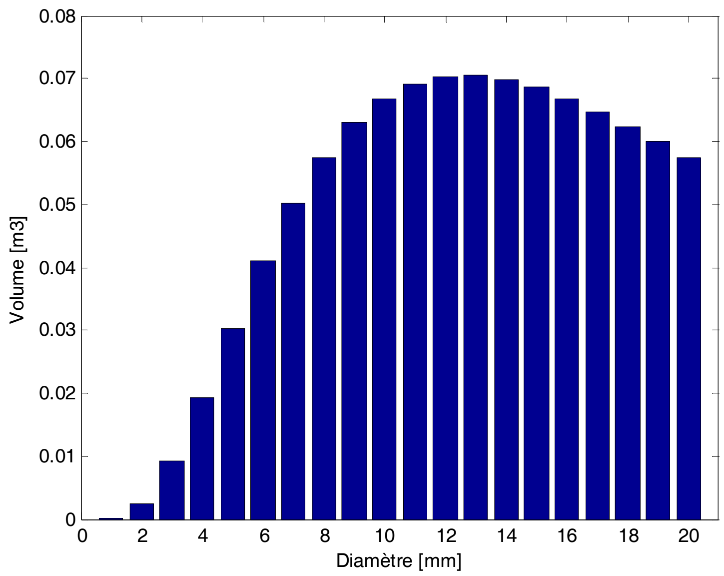
Source: BEAMer
CEPPOL: Centre d'Expertises Pratiques de Lutte Antipollution

Example

Modelling a leak of butanol from a chemical tanker

1. **Modelling the leak rate: tank emptied in 1h44**
2. **Dispersion in the water column**
    1. Number of droplets per diameter group for 1m3 of substance released
    2. Distribution of volume per group for 1m3 of substance released



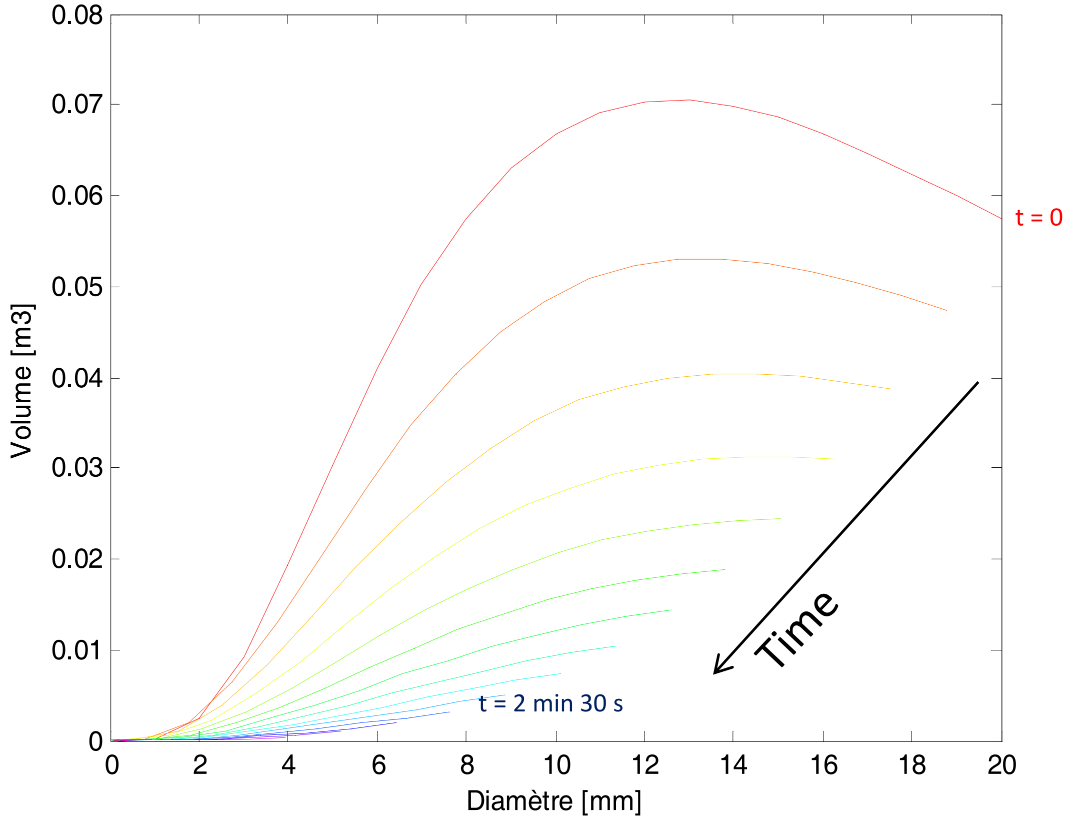


Example

Modelling a leak of butanol from a chemical tanker

1. Dissolution of the different droplet groups

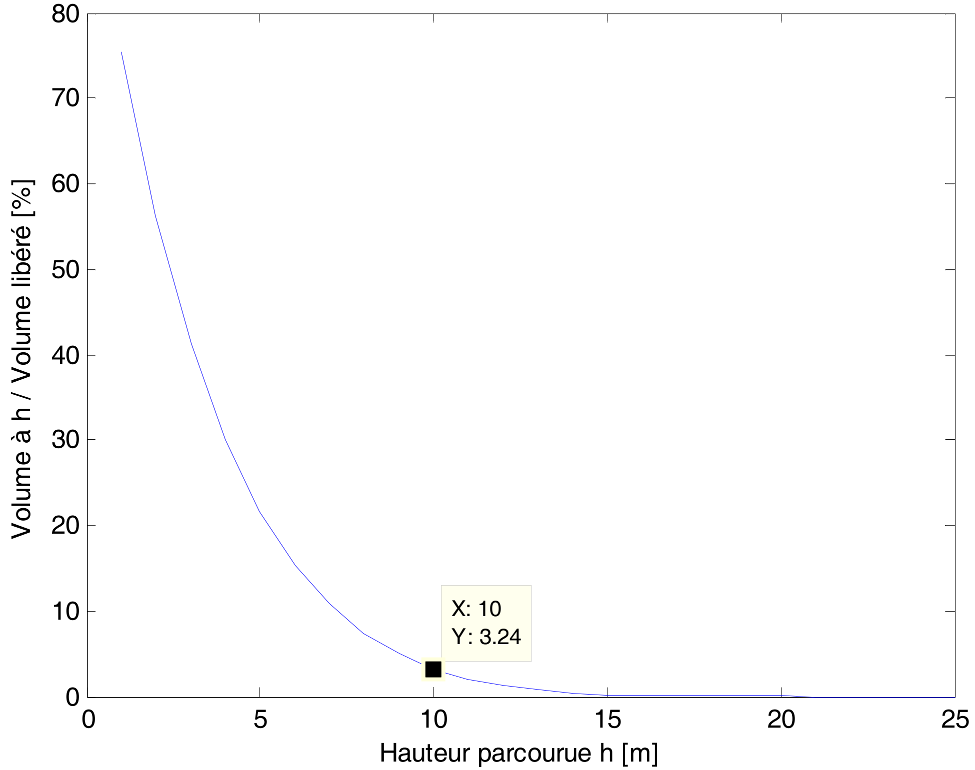
- Evolution of volume over time (Δt = 15 s)



Example

Modelling a leak of butanol from a chemical tanker

Evolution of proportion of initial volume remaining with height



After 10 m: 96% of total volume is dissolved
After 20 m: the butanol is completely dissolved

The future

Modelling dispersion of chemicals at sea

- Consideration of other mechanisms
  - Settling
  - Bioaccumulation
  - Volatilisation

- Consideration of environmental parameters
  - Water temperature
  - Salinity
  - Hydrostatic pressure

Thank you for your attention