



**13th Information Day - Cedre
Hazardous pollution by HNS**

Aerial modelling

Dispersion mechanisms and simulation

*Thibauld Pénelon – INERIS / Accident Risk Division
Explosion-Dispersion Unit - thibauld.penelon@ineris.fr*



*maîtriser le risque |
pour un développement durable*

Presentation plan

Introduction

- Dispersion of a hazardous material in the atmosphere

Atmospheric dispersion - Main mechanisms and impact parameters

- Characterisation of the release of pollutant
- Impact of cloud density
- Impact of meteorological and orographic parameters

Atmospheric dispersion - Models

- Gaussian
- Integral
- Complex (CFD)

Introduction (1/3)

Dispersion of a hazardous material in the atmosphere



EMISSION

(Accidental) release
or « source term »

- gas or liquid jet
- instantaneous release (liq/gaz)
- evaporating pool
- fire smokes...

Atmosphere (humid air)

- meteorological conditions
- sea surface (waves)
- coastal zone...

TRANSPORT DIFFUSION (Dispersion)

Toxic effects
(inhalation, ingestion)

Thermal effects
(ignition)

Pressure effects
(explosion)

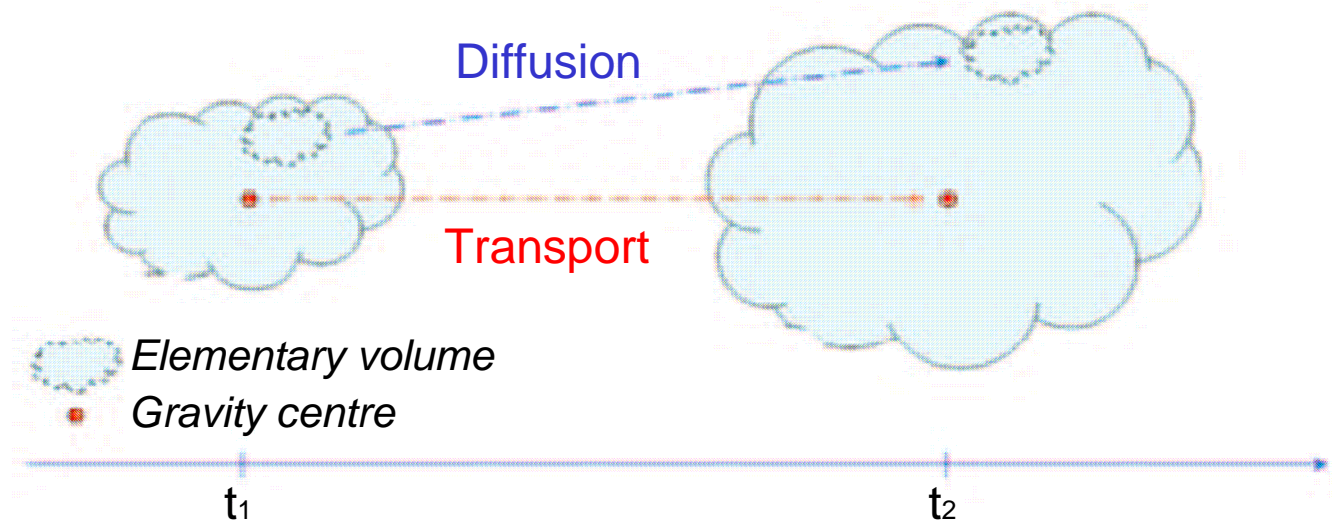
Targets/stakes

- Human (emergency services, coastal population...)
- Environnemental

Introduction (2/3)

Dispersion of a hazardous material in the atmosphere

Transport and diffusion



Representation of the atmospheric dispersion process

(from F. Jourdain, 2007 - Techniques de l'Ingénieur)?

Transport : by wind, depending on cloud density, initial velocity of release

Diffusion : by atmospheric turbulence (surface friction, thermal gradient)



Introduction (3/3)

Dispersion of a hazardous material in the atmosphere

Main impact parameters

- Wind profile and surface roughness
- Thermal gradient (atmospheric stability)
- Obstacles & topography (ships, coastal zone...)
- Characterisation of material and release



Dispersion of a hazardous material in the atmosphere

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- **Characterisation of material and release**

Characterisation of source term (1/2)

Types of emissions

- Storages at ambient pressure
 - liquide material at ambient temperature
(saturated vapour pressure < 1 atm, at T_{amb} - ex. : styrene, xylene, benzene)
 - refrigerated liquefied gas (ex. : NH₃ at -43°C, LNG at -162°C)

⇒ LIQUID RELEASES



Pressurised storage

- pressurized liquefied gas (ex : LPG) ⇒ TWO-PHASE
- gas under pressure ⇒ GASEOUS



Navire transporteur de gaz équipé de citernes pressurisées

- Fire emitting smokes

⇒ GASEOUS RELEASE + soot

LNG pool fire over water
(Gaz de France)

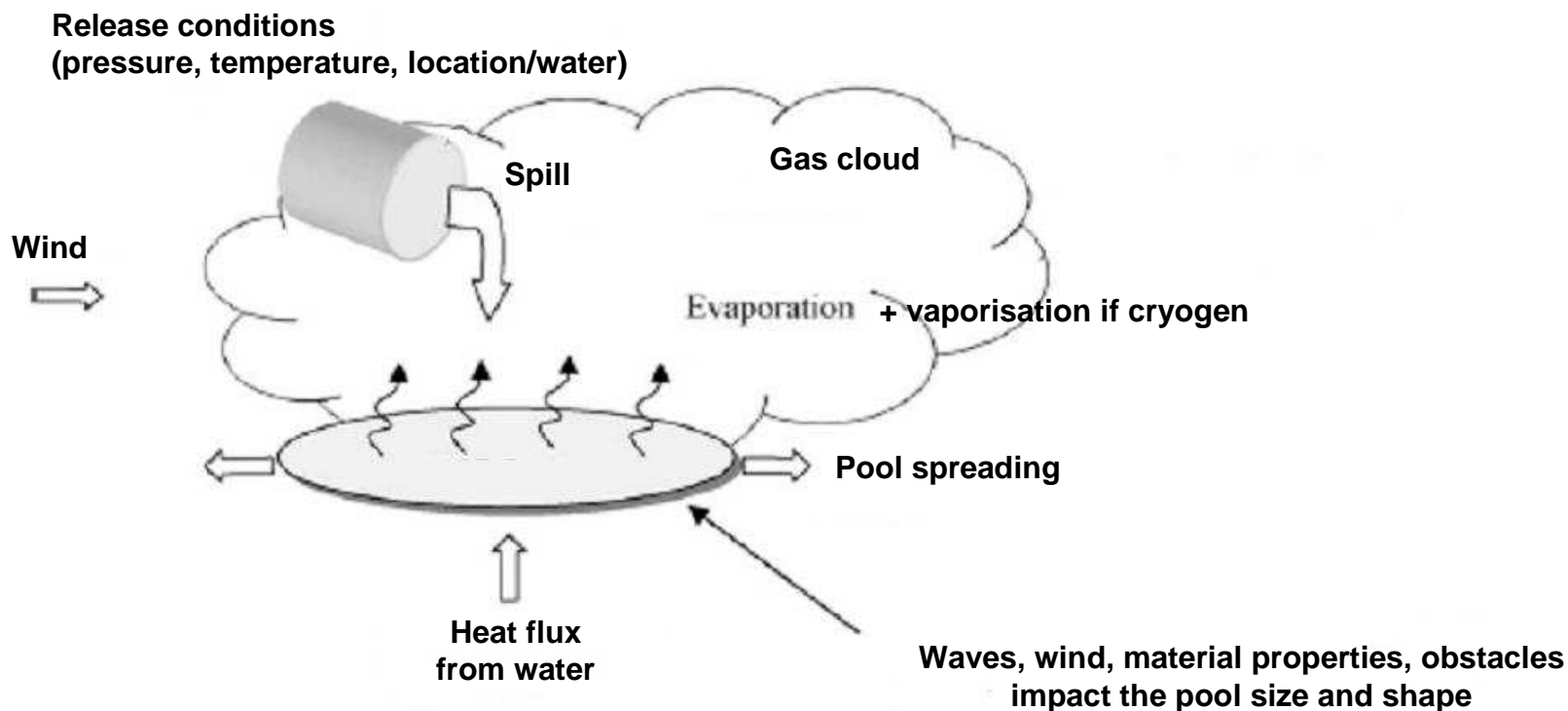


Oil-tanker Limburg (10/2002)
Cargo fire



Characterisation of source term (2/2)

- Instantaneous release (sudden aperture of a tank)
- Continuous release (long-lasting leak on a tank)



(From Luketa-Hanlin, 2006)

Illustration - Release of liquefied gas over water



Impact of the density of released materials

> Passive gas

> Dense gas

> Buoyant gas

Origin?

- Same density as air
- Very diluted with air
- no inertial jet

- High density at T_{amb} (Cl_2 , $COCl_2$...)
- Two-phase release (pressurized LPG)
- Cooled gas

- Low density at T_{amb} (H_2 , CH_4 , NH_3 gas...)
- hot gases (fire smokes...)

Consequences?

- Transport at wind velocity
- Dilution by atmospheric turbulence

- Gravity effects
⇒ collapse
⇒ increased dilution at cloud lateral faces
- Higher surface friction
- High concentrations at surface level

- Elevation
- Increased dilution by wind shear
- Lower concentrations at surface level



Illustration - Release of liquefied ammonia

- Movie : Release of ammonia in free field (over flat terrain)
INERIS Trials, 1997 (movie Trial 2)

TRIAL N°2

Horizontal free jet \varnothing 20 mm

ESSAI N°2

Jet libre horizontal \varnothing 20 mm



Dispersion of a hazardous material in the atmosphere

Main impact parameters

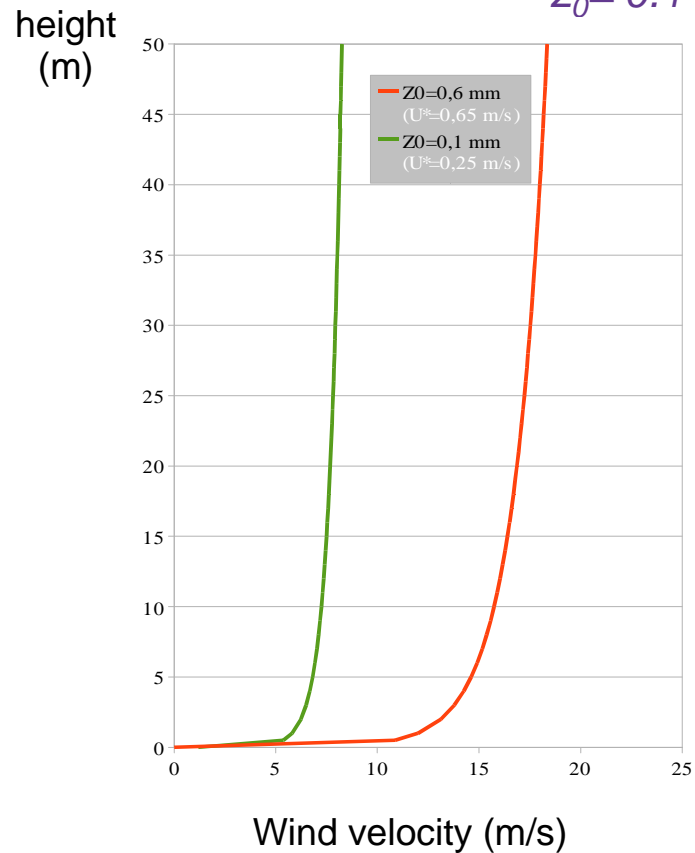
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Wind velocity and surface roughness length (sea)

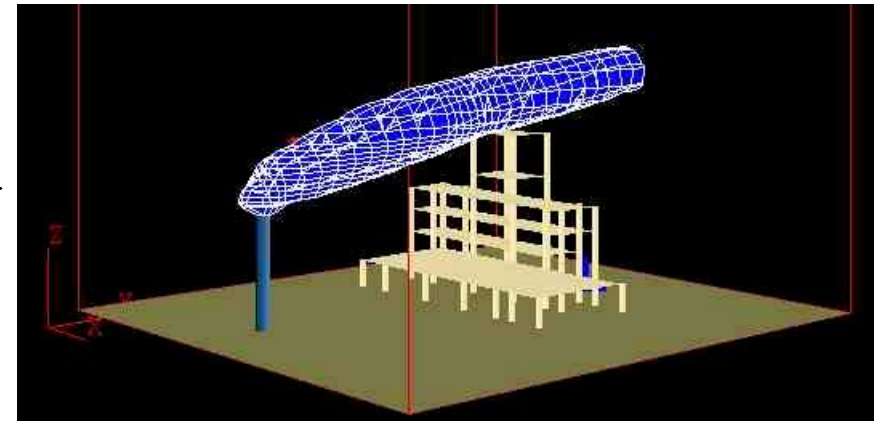
Vertical wind profile typically logarithmic / depending on surface roughness

Open water surface roughness depend on waves, thus on wind shear

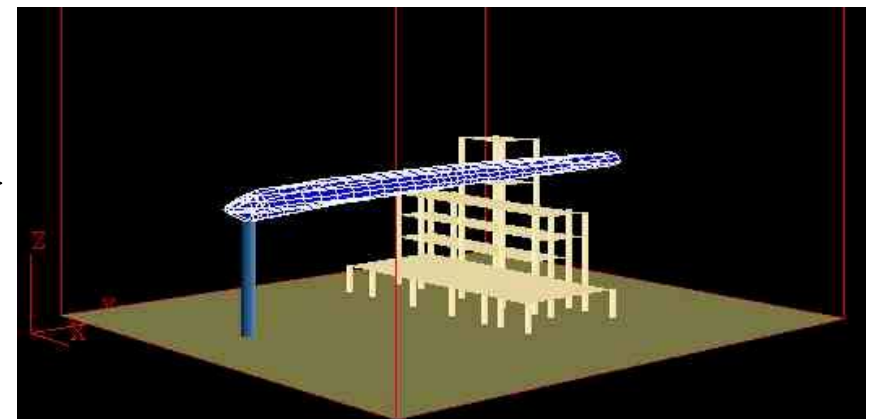
$z_0 = 0.1$ à 0.6 mm according to Brutsaert (1982)



3 m/s



10 m/s



The more wind, the more dilution (impact of shear)



Dispersion of a hazardous material in the atmosphere

Main impact parameters

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Atmospheric stability \Leftrightarrow vertical temperature gradient

- P_{atm} decreases with height : cooling of the air

When?

Neutral atmosphere

Day/night transition
High cloud cover
Strong wind

Consequence?

Rising air mass "stays at its new location"

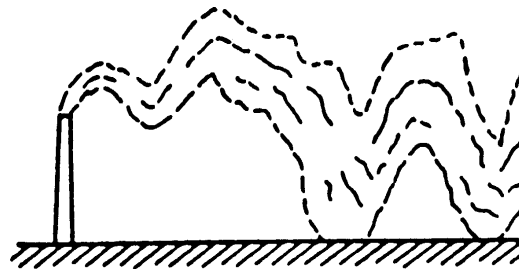
Mean turbulence intensity
 \Rightarrow "normal" dilution
(Class of Pasquill D)

Unstable atmosphere (or "convective")

Sunny day, low wind
(surface heated by solar radiation)

Rising air mass warmer than the air around

\Rightarrow goes on rising
High turbulence intensity
 \Rightarrow **high dilution**
(Classes of Pasquill A to C)

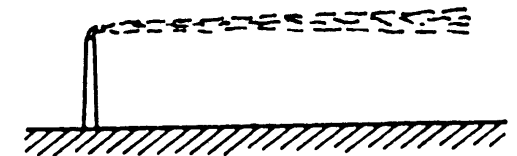


Stable atmosphere

Clear night, low wind
(surface cooling faster than the air above)

Rising air mass cooler than the air around

\Rightarrow back to initial position
Low turbulence intensity
 \Rightarrow **Low dilution**
(Classes of Pasquill E and F)





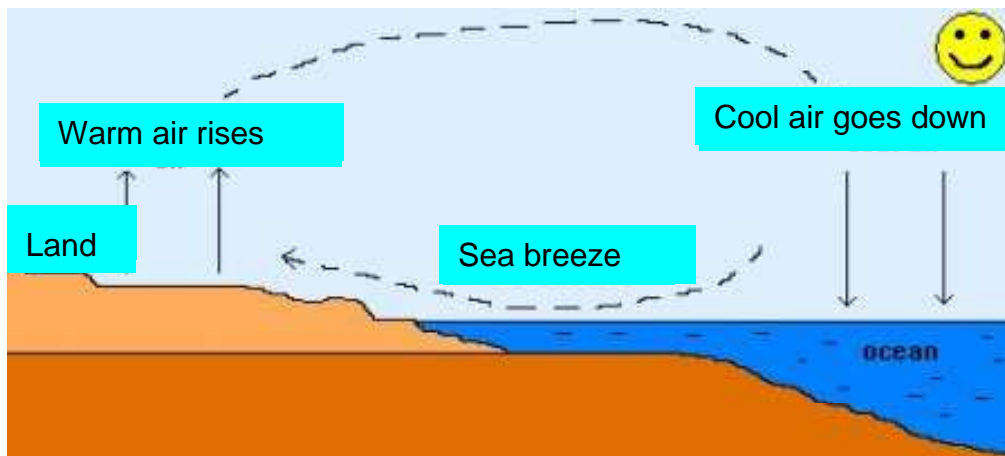
Dispersion of a hazardous material in the atmosphere

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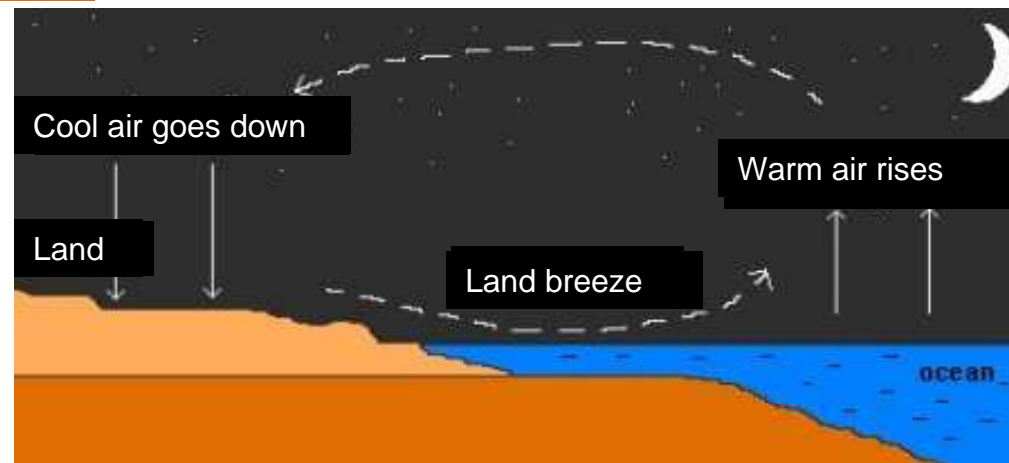
Coastal zone : littoral breezes

Thermally induced turbulence



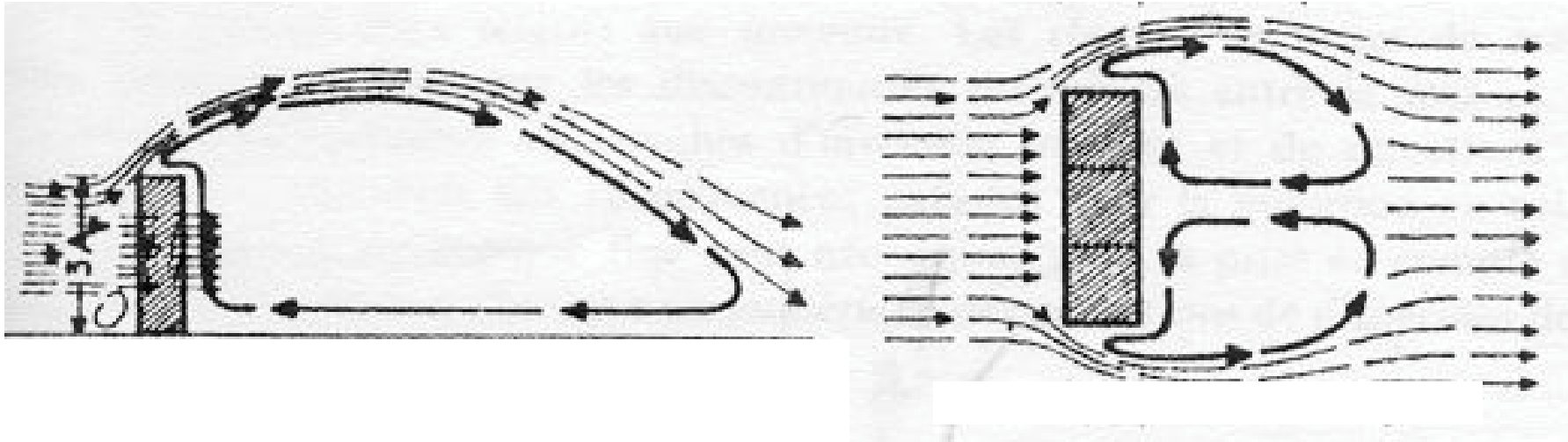
Sea breeze

Land breeze



Presence of an obstacle (ex. : ships nearby)

Mechanically induced turbulence - Wake effects



INERIS Trials, 1997 (movie Trial 5)



Accidental aerial dispersion models (near field / short term)

GAUSSIAN

Dispersion driven
only by meteo
conditions !

Validity
 $100\text{ m} < d < 10\text{ km}$

INTEGRAL

« Over » simplified
equations of
fluid mechanics !

Validity
 $20\text{ m} < d < 10\text{ km}$

« 3D » ou CFD

Less simplified
equations of
fluid mechanics...

Validity
 $1\text{ cm} < d < 10\text{ km}$

Gaussian-type models

Principle

- Solution of dispersion equation = gaussian distribution law

Applications

- Passive gas
- Emergency situations

Simplified hypotheses and limits

- Neglect molecular diffusion
- Uniform wind field (speed and direction) in time and space
- No obstacle / no relief...
- Not adapted for heavy gas dispersion

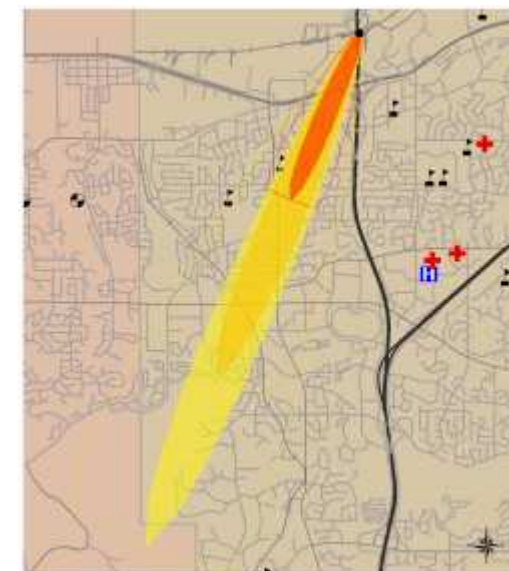
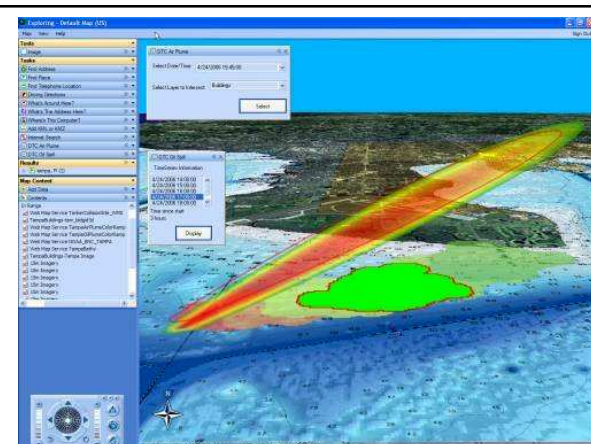
Examples

ALOHA (EPA/NOAA) (+ *integral model for dense gas (DEGADIS)*)

EPIcode (Homann Associates, Inc.)

INPUFF (EPA) (*multisource + adaptation for light gases*)

...



Integral-type dispersion models

Principle

- Simplified resolution of fluid mechanics equations
- Setting of parameters in order to obtain conservative hazardous distances

Applications

- Passive gas, heavy/dense gas, and sometimes buoyant gas

Hypotheses

- Several successive models (jet model, heavy gas model, buoyant gas model...)
- Gaussian model used for the final (passive) dispersion phase

Limitations

- Conservative parametric approach
- Gaussian model limits (constant meteorological conditions, neither relief nor obstacles)
- Not adapted to low wind/laminar release (no molecular diffusion considered)

Examples

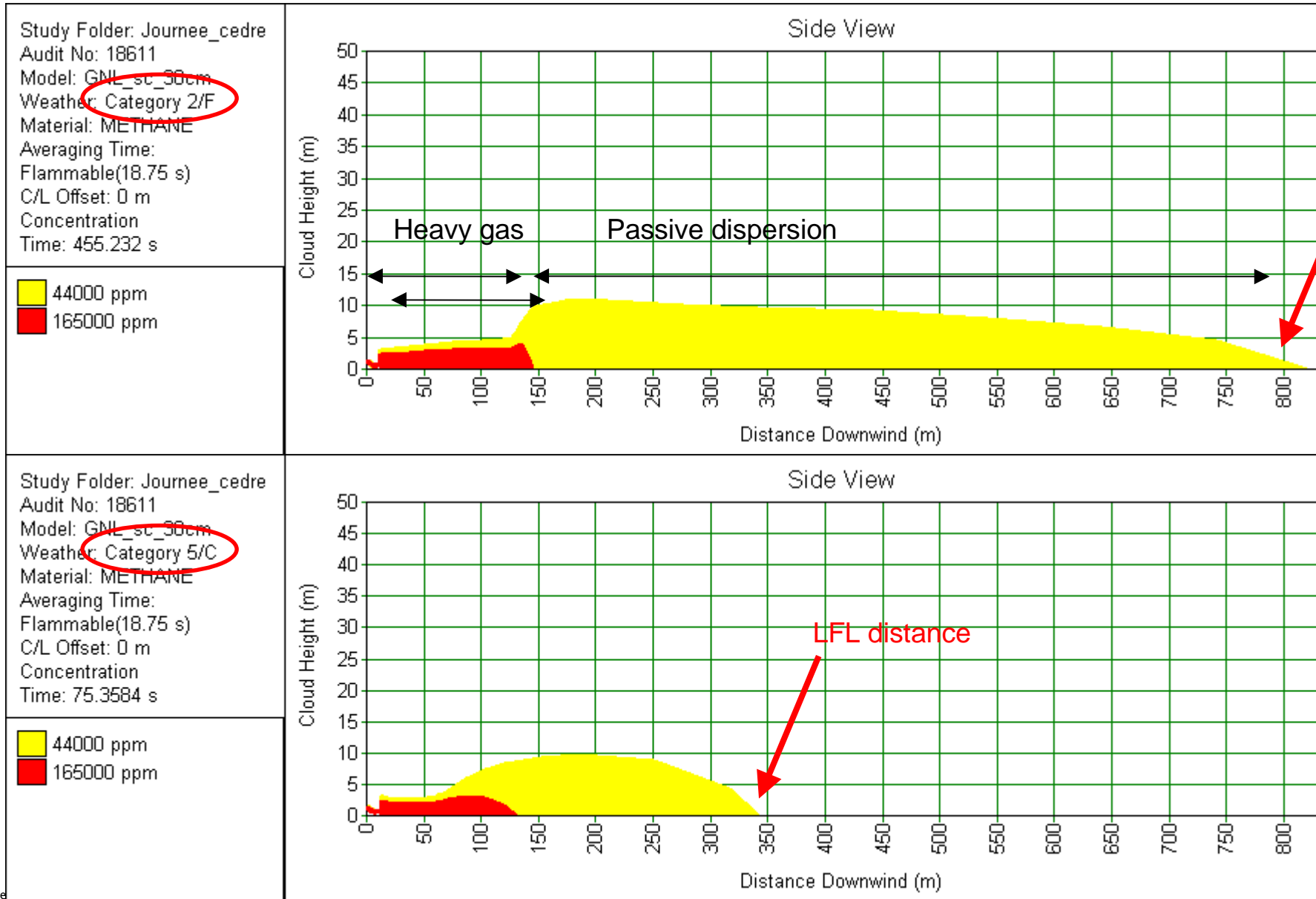
EFFECTS (TNO, Pays-Bas)

SAFER (Safer Systems, USA)

PHAST (DNV Software, UK)

SEVEX (Atm-Pro / Faculté Polytechnique de Mons, Belgique)...

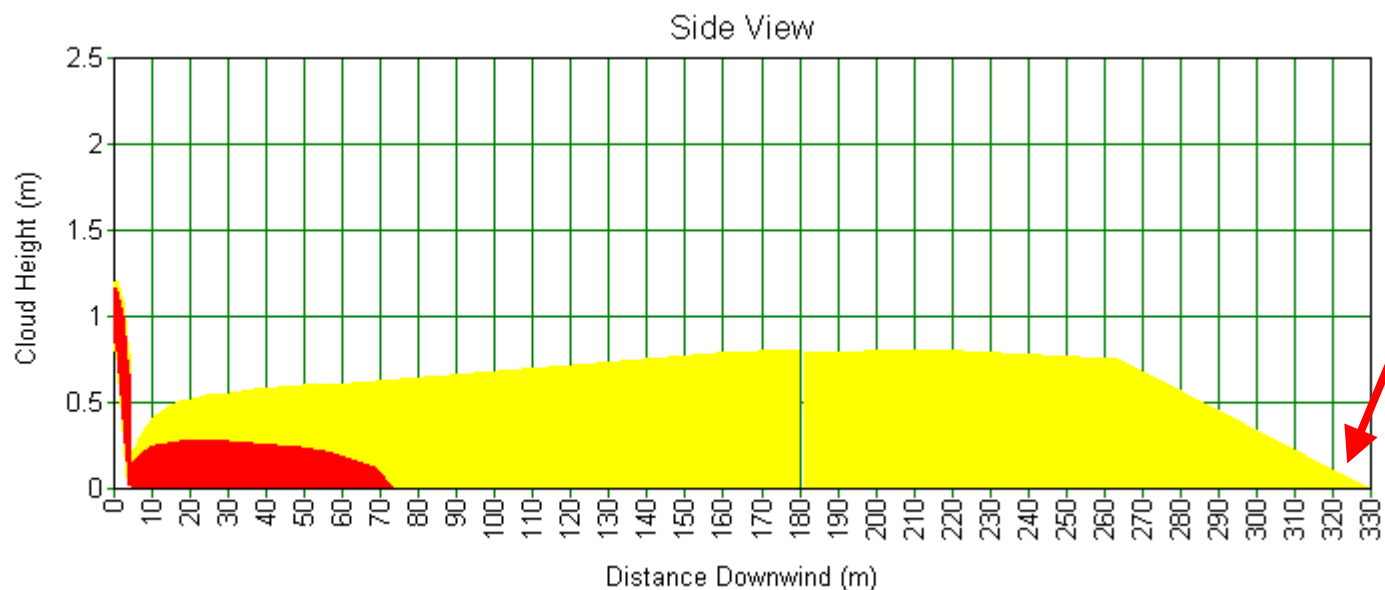
Example : simulation of aerial dispersion of LNG over water with Phast



Exemple : simulation of aerial dispersion of Xylene over water with Phast

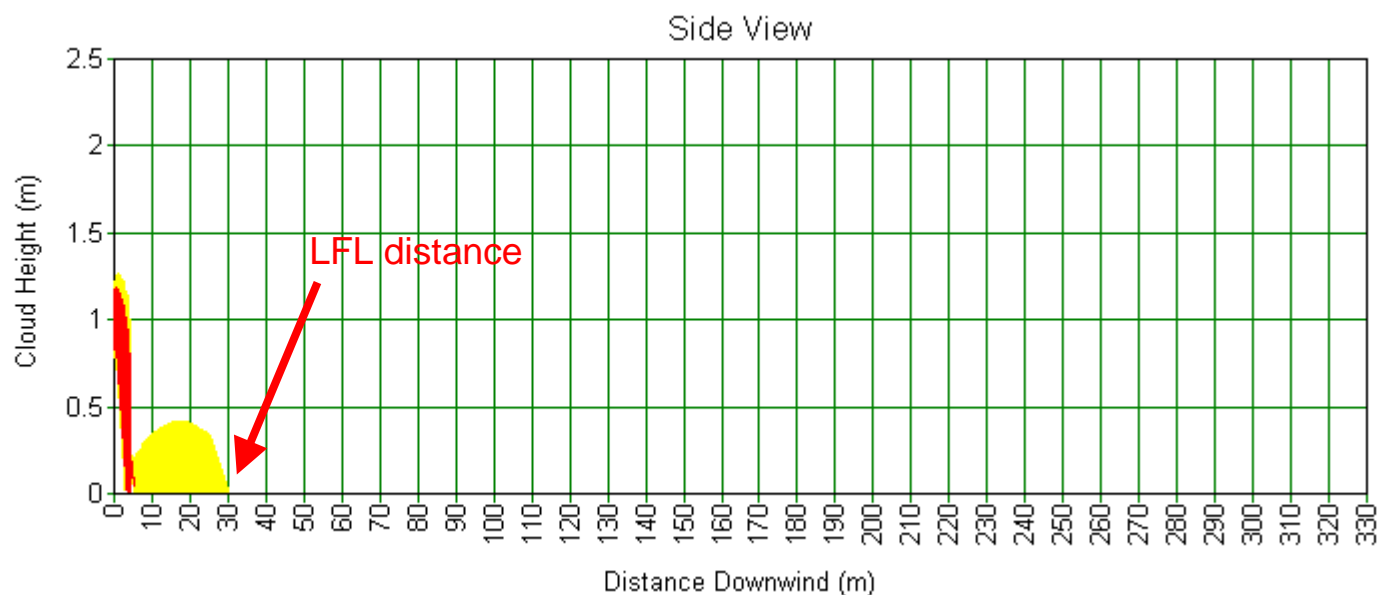
Study Folder: Journee_cedre
Audit No: 19521
Model: Xylene_sc10_2.5dm
Weather: **Category 2/F**
Material: M-XYLENE
Averaging Time:
Flammable(18.75 s)
C/L Offset: 0 m
Concentration
Time: 3574.87 s

11000 ppm
70000 ppm



Study Folder: Journee_cedre
Audit No: 19521
Model: Xylene_sc10_2.5dm
Weather: **Category 5/C**
Material: M-XYLENE
Averaging Time:
Flammable(18.75 s)
C/L Offset: 0 m
Concentration
Time: 3461.36 s

11000 ppm
70000 ppm



CFD-type models

Principle

- « Complete » resolution of fluid mechanics equations

Applications / Hypotheses

- Turbulent fluctuations, obstacles and relief
⇒ Simulation of complex environments
- If stakes request to refine the evaluation (expensive)

Limitations

- Numerous input and numerical parameters
 - CPU time consuming
 - Accuracy depends on resolution method, grids, selected models...
- expensive

Examples

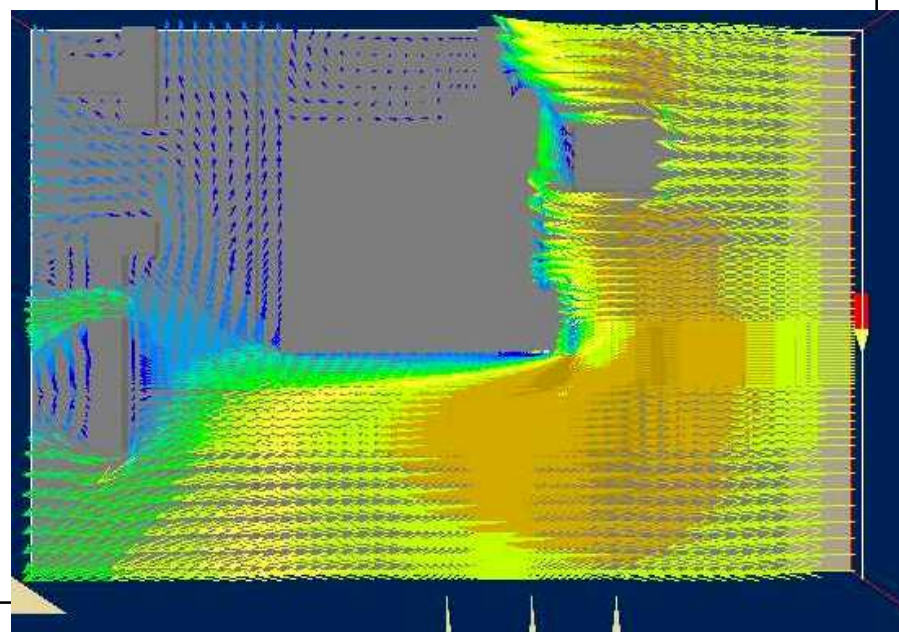
CFX, Fluent (Ansys) - *Generalist*

PHOENICS (Cham) - *Generalist*

Mercure (EdF) - *Atmospheric dispersion*

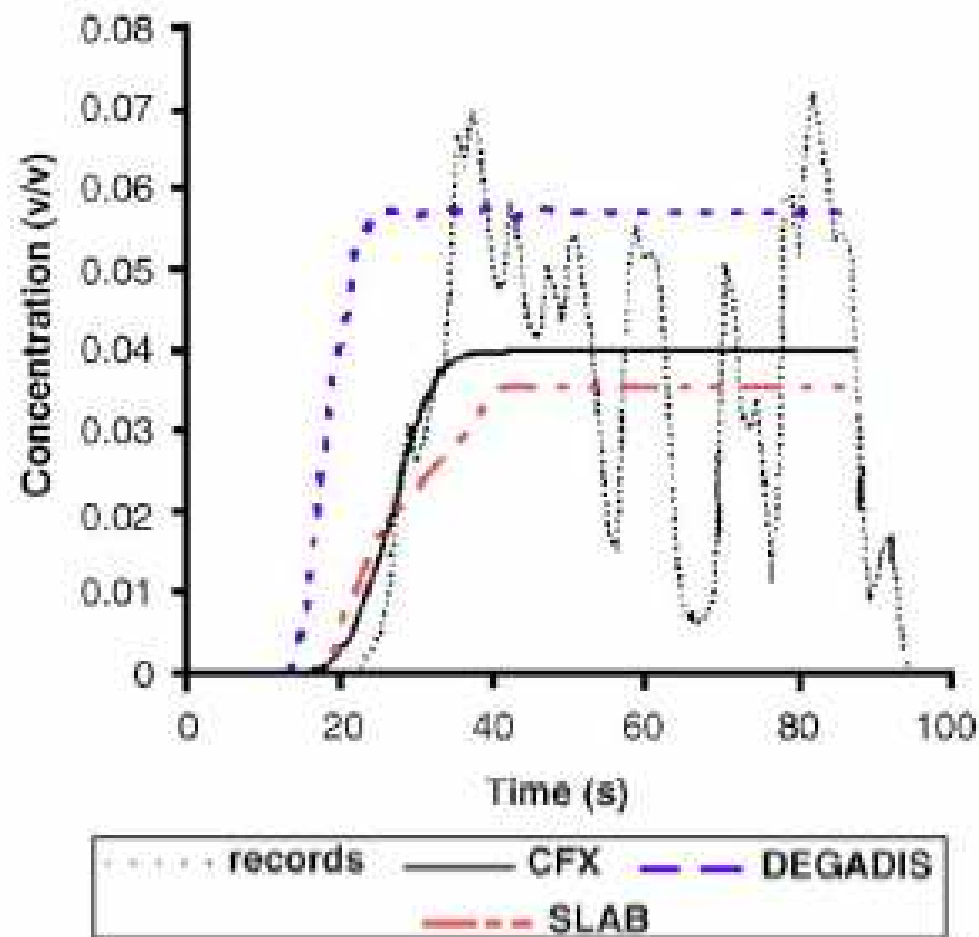
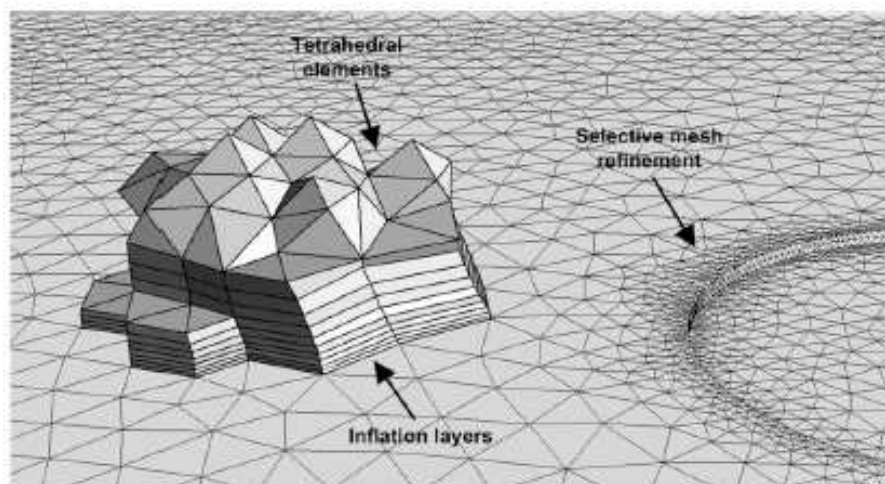
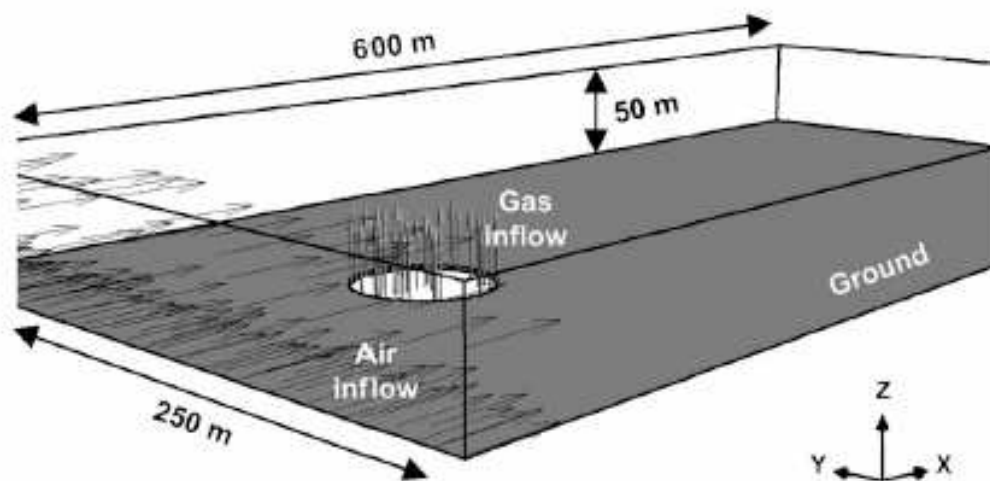
FLACS (GexCon) - *Dispersion and explosion*

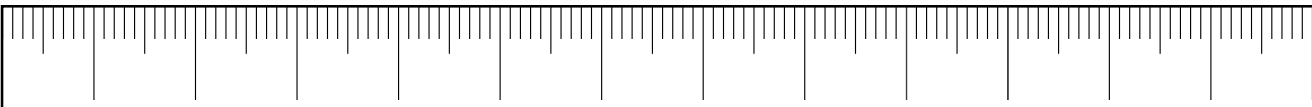
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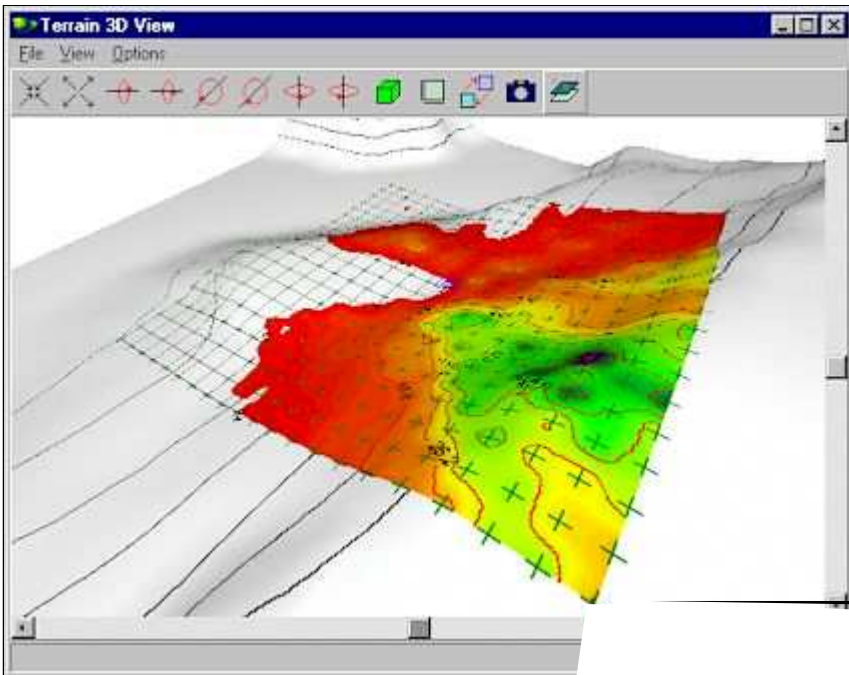


Example of comparison of CFD and integral models

Liquefied Natural Gas pool evaporation and atmospheric dispersion
(d'après Sklavounos & Rigas, 2006)





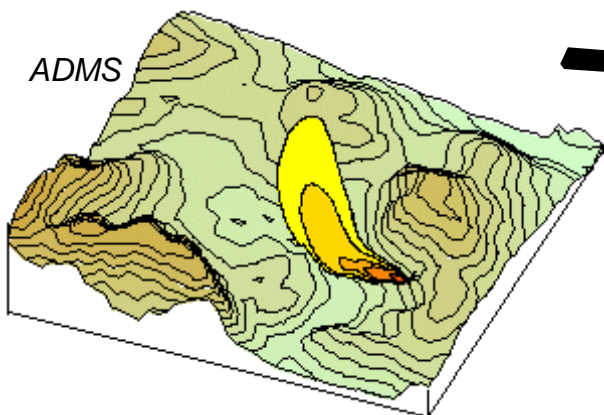


ISC-AERMOD View

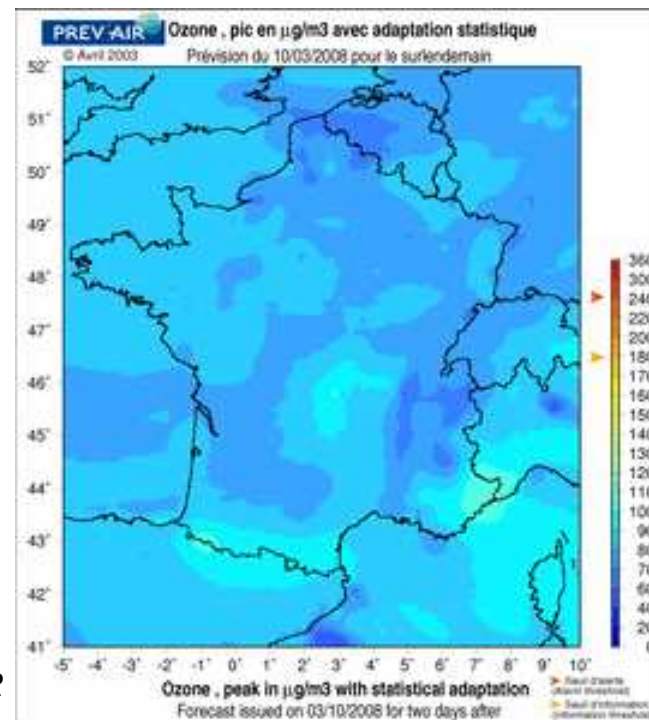
Breeze
CALPUFF



Thanks for
your attention



ADMS



PREV AIR