18th *Cedre* Information Day
Spill modelling

Atmospheric dispersion models

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maîtriser le risque
pour un développement durable

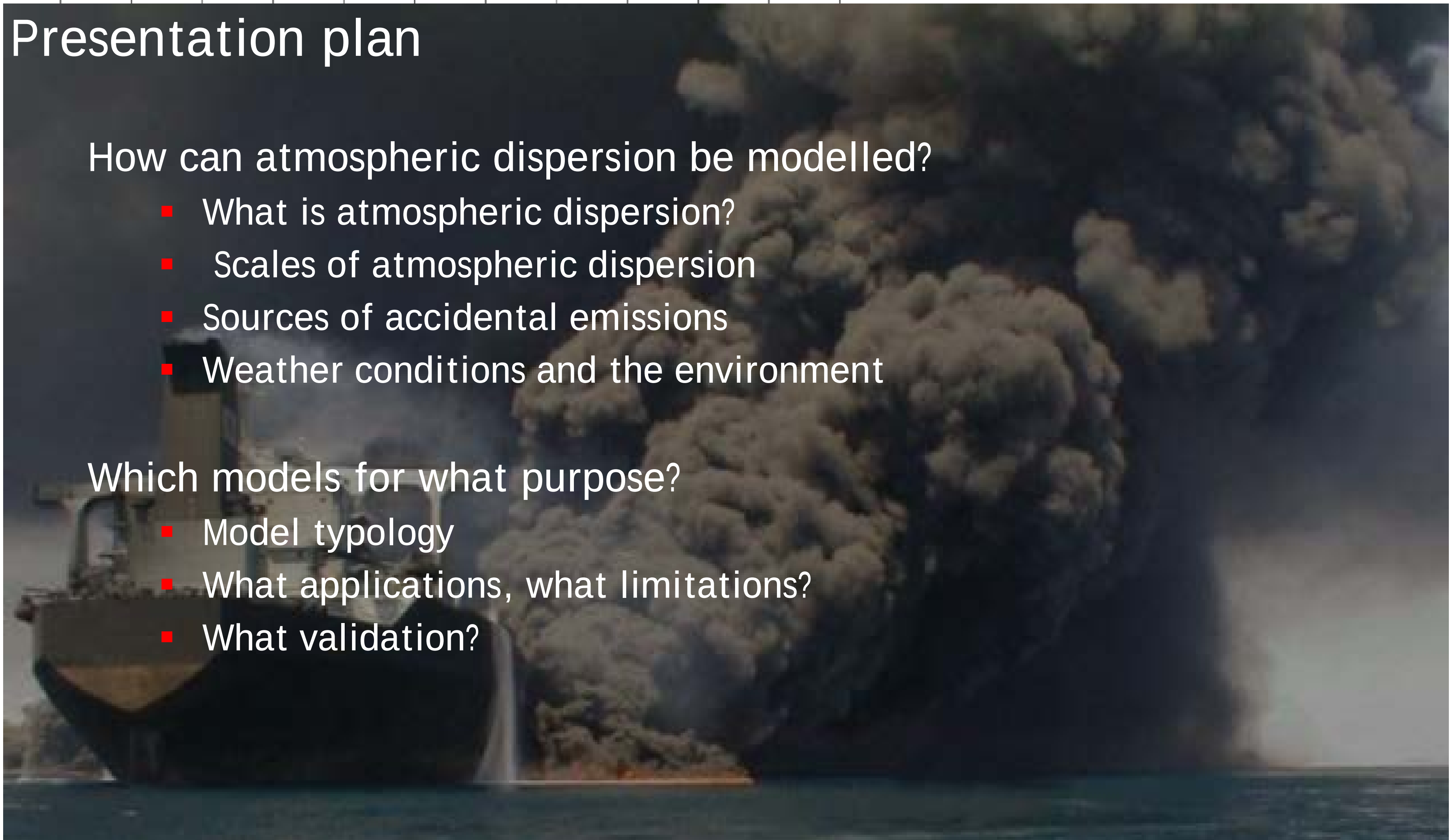
Presentation plan

How can atmospheric dispersion be modelled?

- What is atmospheric dispersion?
- Scales of atmospheric dispersion
- Sources of accidental emissions
- Weather conditions and the environment

Which models for what purpose?

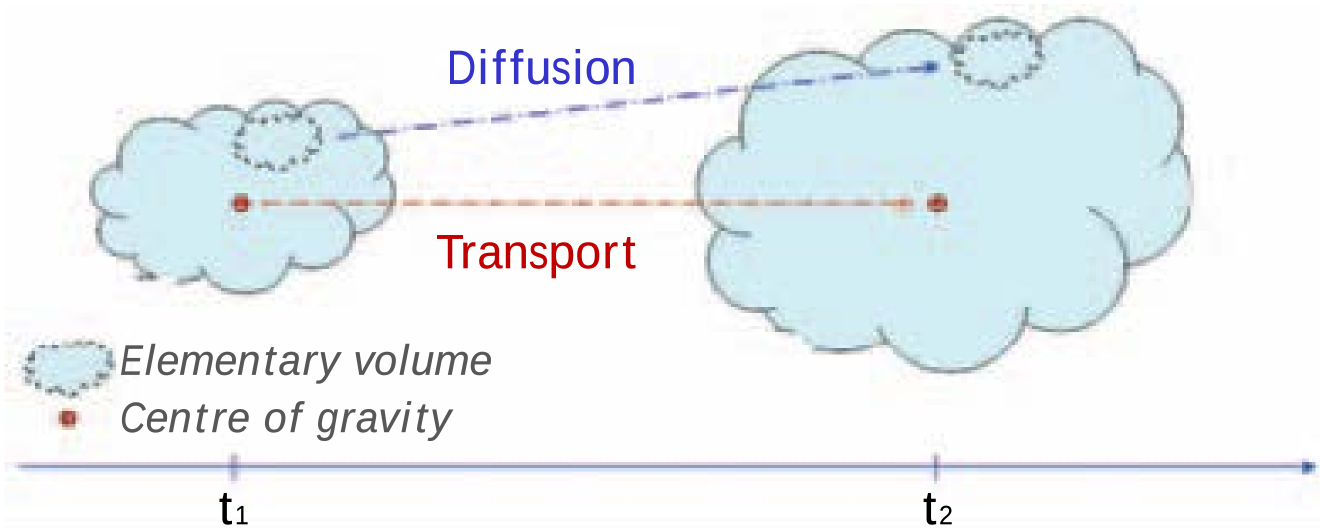
- Model typology
- What applications, what limitations?
- What validation?



Following the attack on the Limburg oil tanker, off Yemen, 2002 – source www.meretmarine.com

What is atmospheric dispersion?

The **transport** and **diffusion** of a quantity of substance in the air



Representation of the atmospheric dispersion process

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

Transport: by the **wind**, according to the cloud's density, initial speed of release

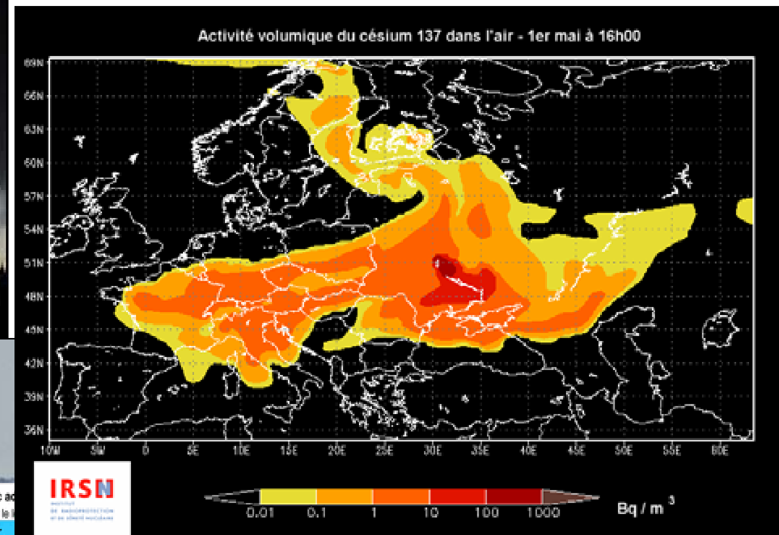
Diffusion: by atmospheric **turbulence** (surface friction, thermal gradient)
by turbulence generated by obstacles

Scales of atmospheric dispersion

INERIS trials

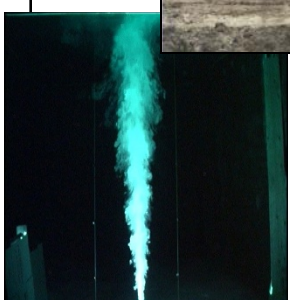
Buncefield - BBC

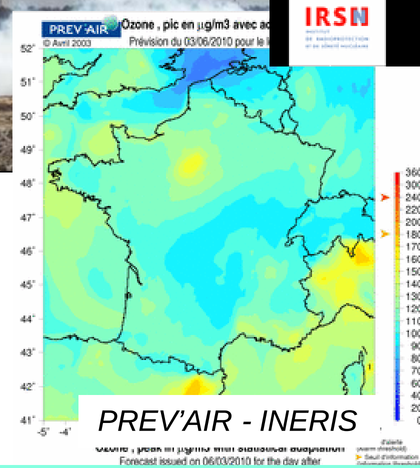
Chernobyl - IRSN



Trials INERIS

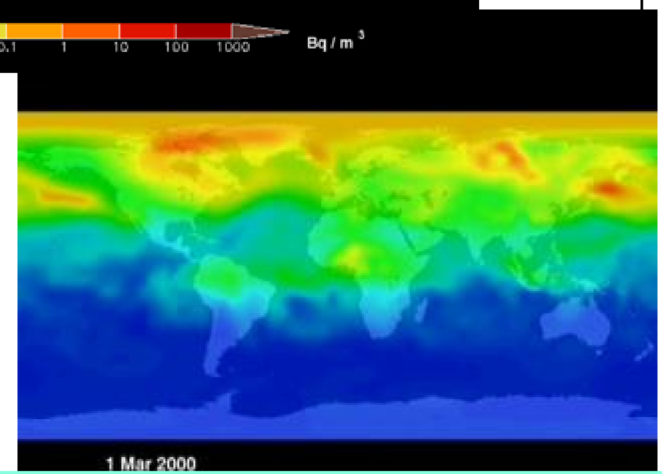
Trials INERIS





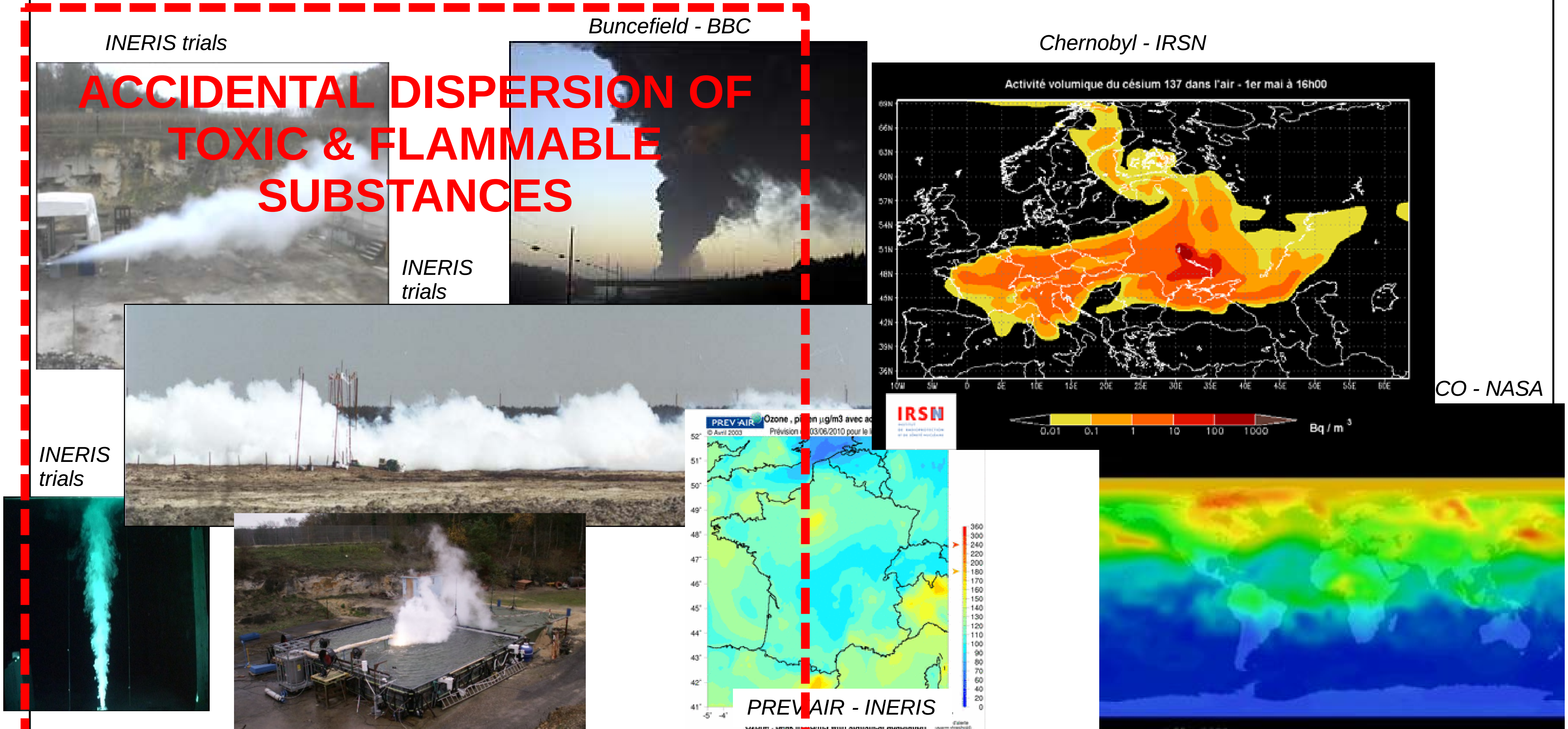
PREV'AIR - INERIS

CO - NASA



Micro	Local	Meso (regional)	Macro, Global (Synoptic)
< 1000 m	~ 100 m-50 km	~ 10-200 km	~ 100-100 000 km
sec – min	min-hours	days	months-years

Scales of atmospheric dispersion



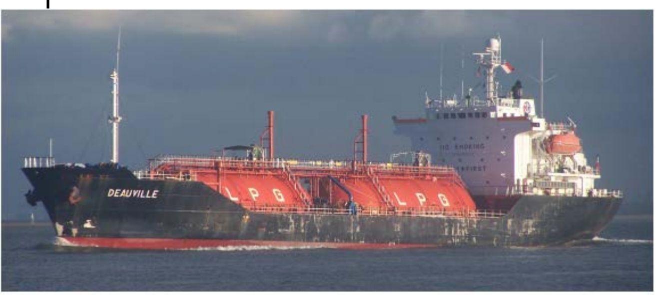
Micro	Local	Meso (regional)	Macro, Global (Synoptic)
< 1000 m	~ 100 m-50 km	~ 10-200 km	~ 100-100 000 km
sec – min	min-hours	days	months-years

To simulate atmospheric dispersion…

A source of emission to be characterised…

- Storage at atmospheric pressure
  - liquid substance at ambient temperature
    (saturated vapour pressure < 1 atm, at T_{amb} - e.g. styrene, xylene, benzene)
  - refrigerated liquefied gas (e.g. NH_3 at -43°C, LNG at -162°C)

  ⇒ LIQUID RELEASE ⇒ VAPOUR EMISSION



Navire transporteur de gaz équipé de citernes pressurisées

- Pressurised storage
  - pressurised liquefied gas (e.g. LPG) ⇒ DIPHASIC
  - pressurised gas ⇒ GASEOUS

- Fire emitting smoke

  ⇒ GAS RELEASE + soot

LNG slick on fire on water
(Gaz de France trials)

Limburg oil tanker (10/2002)
Cargo fire

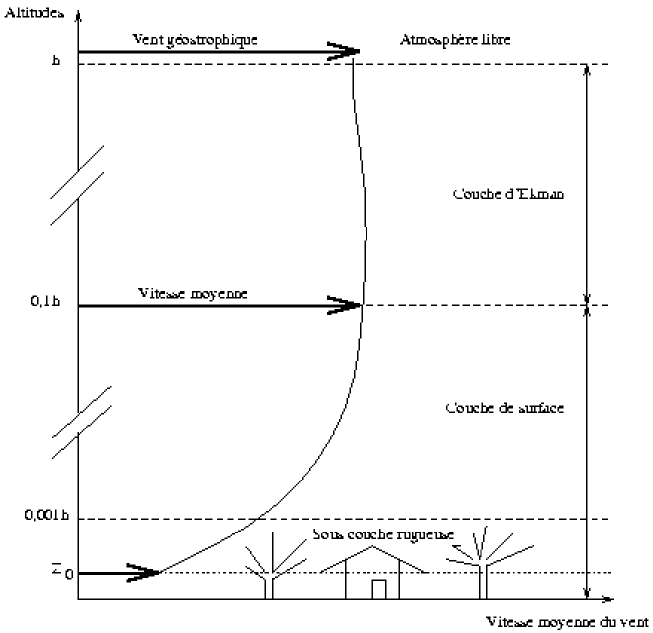
To simulate atmospheric dispersion…

… atmospheric conditions to be defined (1/5)

Atmospheric boundary layer

> surface layer (0-100m) characterised by:

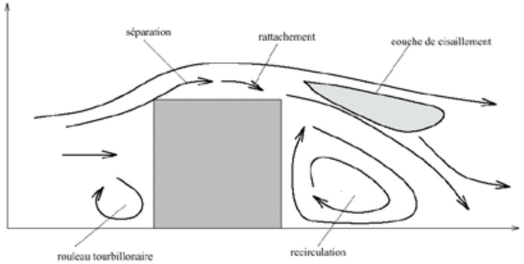
- The average wind field
- The temperature field
- The turbulence (atmospheric stability)



- Parameters influenced by the environment
  - ✓ Relief
  - ✓ Obstacles
  - ✓ Surface type

    (roughness depending on sea state, land occupation)

    (thermal)



To simulate atmospheric dispersion…

… atmospheric conditions to be defined (2/5)

ON LAND

When?

Consequence?

Neutral atmosphere

Day/night transition

Heavy cloud cover

Strong wind

moving air mass
"<u>stays at its new location</u>"

moderate turbulence

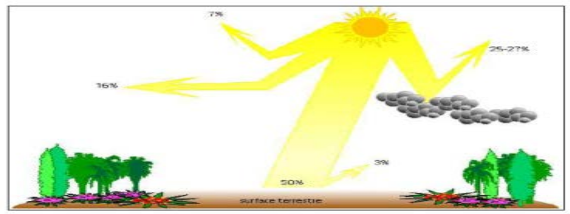
⇒ "normal" dilution

(Pasquill class D)

Unstable atmosphere (or "convective")

Sunny day, low wind

Ground heated by sun's rays



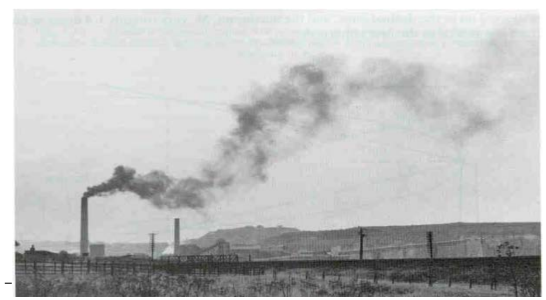
moving air mass warmer than the air around

⇒ <u>rises further</u>

High turbulence

⇒ high dilution

(Pasquill classes A to C)



Stable atmosphere

Clear night, low wind

Ground cooling faster than the air

moving air mass cooler than the air around

⇒ <u>back to initial position</u>

Low turbulence

⇒ low dilution

(Pasquill classes E and F)

To simulate atmospheric dispersion…

… atmospheric conditions to be defined (3/5)

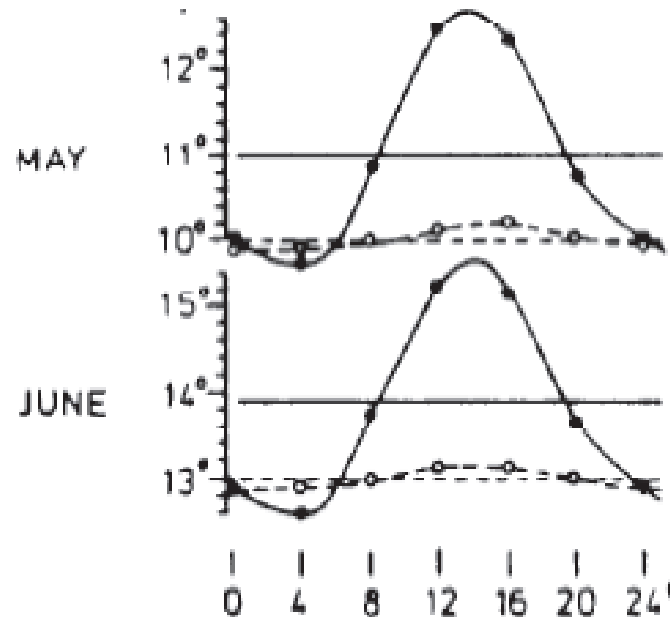
AT SEA

At sea, surface temperature variations are very low during the diurnal cycle (ΔT < 1°C at sea; ΔT up to 20°C on land!)

⇒Water surface/ambient air temperature gradient often lower than on land

⇒Opposite to stability conditions on land:

- moderately unstable
  - mainly at night
- slightly stable
  - mainly during the day
- neutral



------- Water temperature

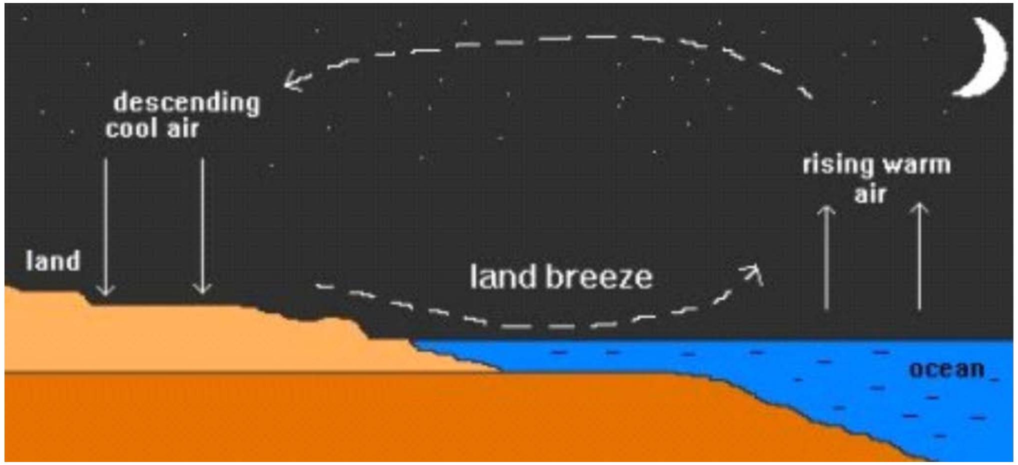
_____ Air temperature

Average diurnal cycle in the North Sea (Hanna, 1984)

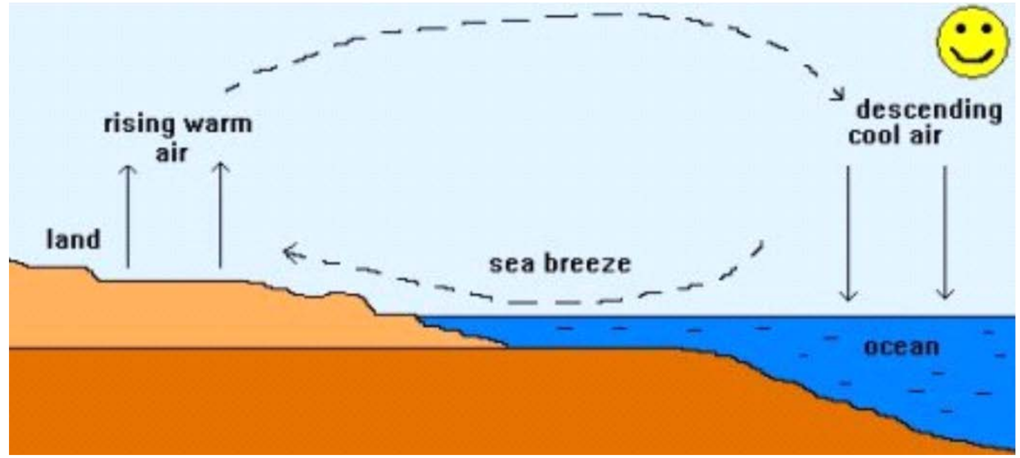
To simulate atmospheric dispersion…

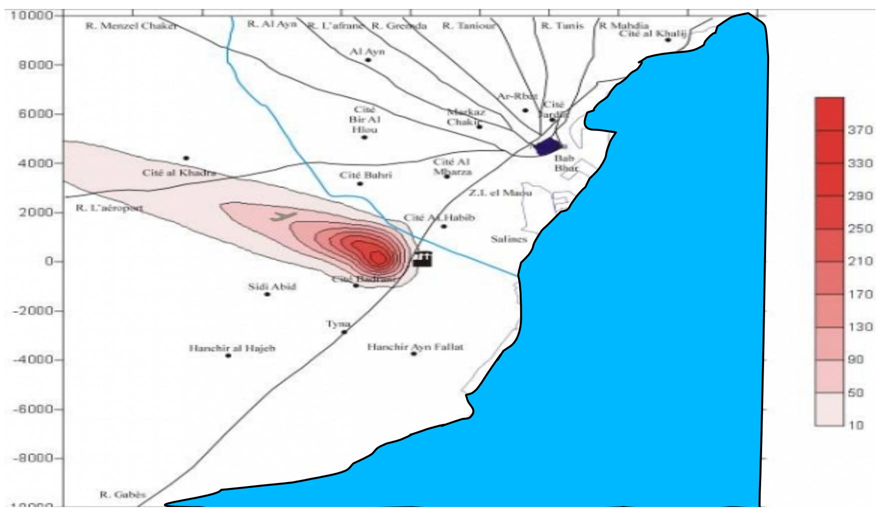
… atmospheric conditions to be defined (4/5): coastal breezes

Land breeze

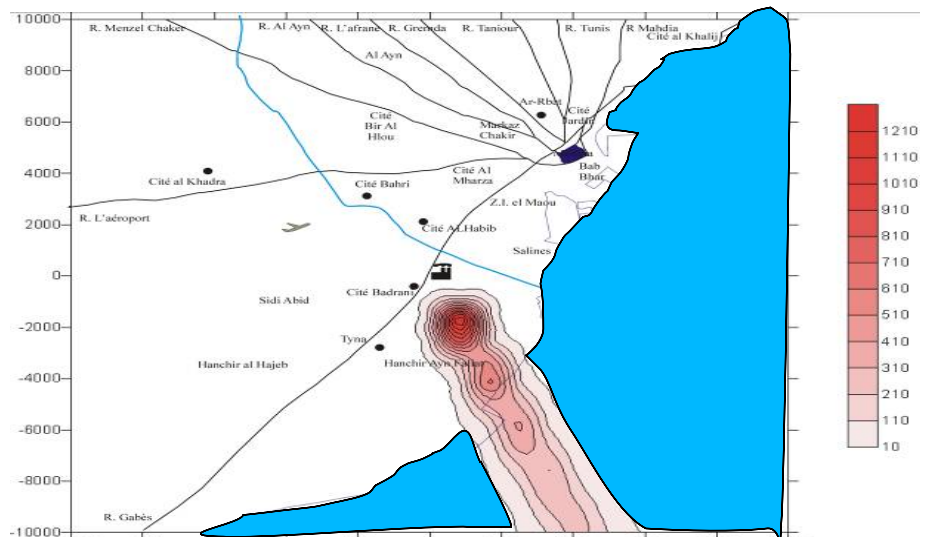


Sea breeze





00:00 - Dispersion of SO2 with sea breeze
(Dahech et al. 2011)



15:00 - Dispersion of SO2 with land breeze
(Dahech et al. 2011)

2013

Aéroport

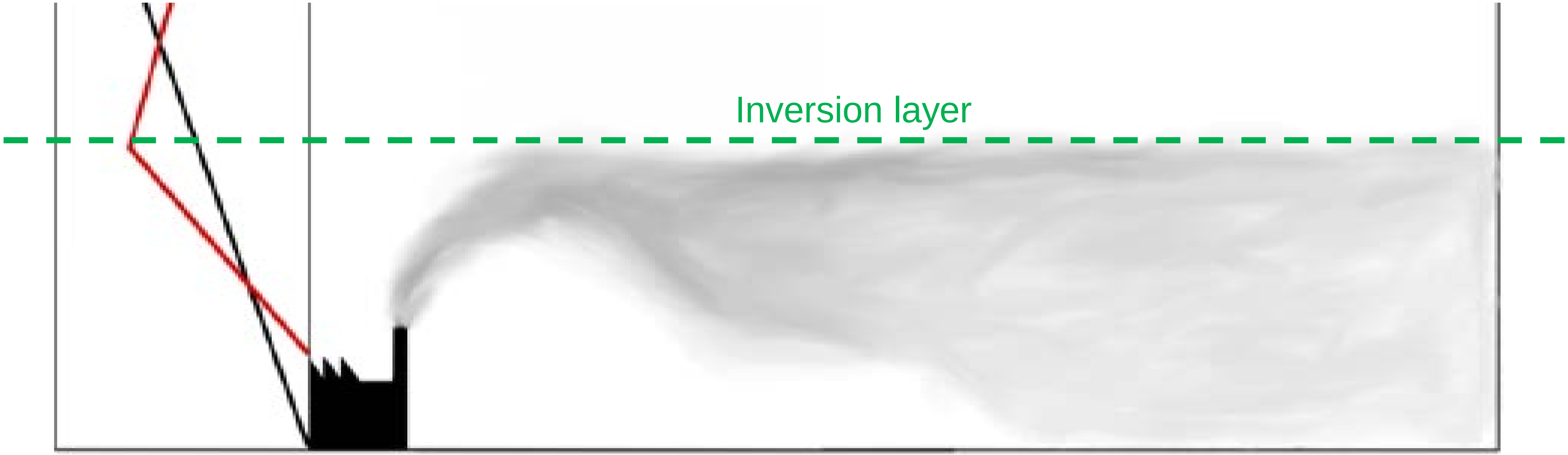
Aéroport

To simulate atmospheric dispersion…

… atmospheric conditions to be defined (5/5): thermal inversion

The "inversion layer" is an area where the temperature rises with altitude (high local atmospheric stability):

Gas emissions are trapped between the ground and the inversion layer (except if the speed of the plume enables it to penetrate the layer e.g. hot smoke...)



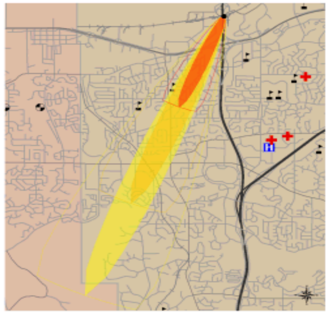
Source : http://courses.washington.edu/cee490/PlumeD4.pdf

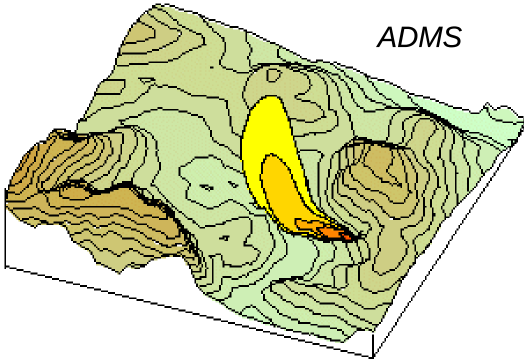
Which models for what purpose?

To understand phenomena
To protect populations and property
To protect the environment

- Prevention: risk reduction at source
  urbanisation control
  emergency services preparation
- Emergency: adequacy of response resources
  to protect people
  (teams, emergency services, population)
  to protect the environment
  to protect property

Dispersion model typology: three approaches





Complexity:

Gaussian model (for passive dispersion)

Dispersion driven by weather conditions alone

Validity: 100 m < d < 10 km

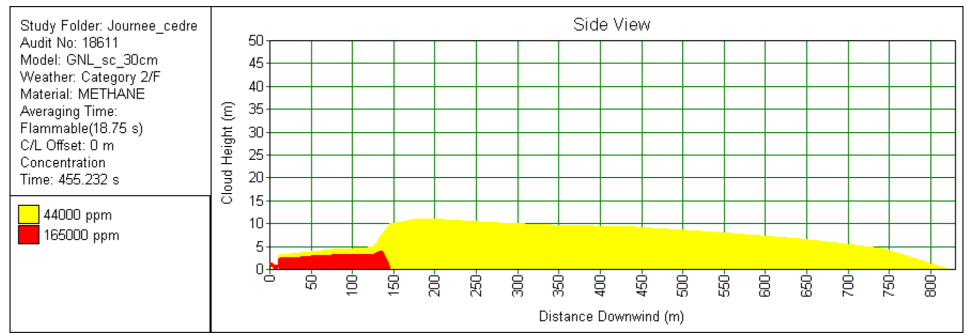
E.g. ALOHA (EPA/NOAA, USA), ADMS (CERC), INPUFF (EPA)…

Integral model (jet, heavy gas...)

Simplified resolution of fluid mechanics equations

Validity: 20 m < d < 10 km

E.g. EFFECTS (TNO), SAFER (Safer Systems), PHAST (DNV Software)….



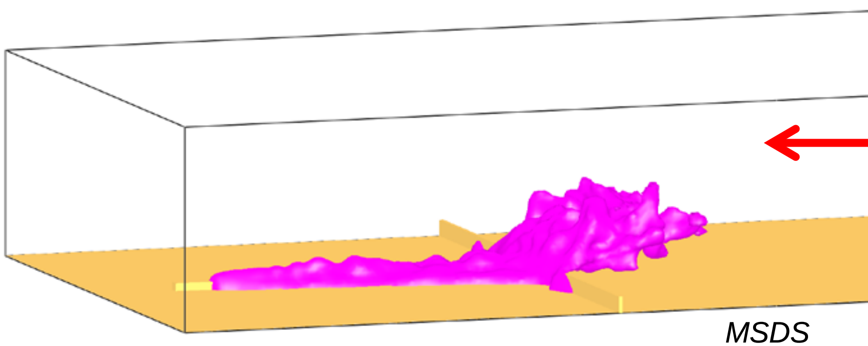
PHAST

CFD model (= Computational Fluid Dynamics)

Fuller resolution of fluid mechanics equations

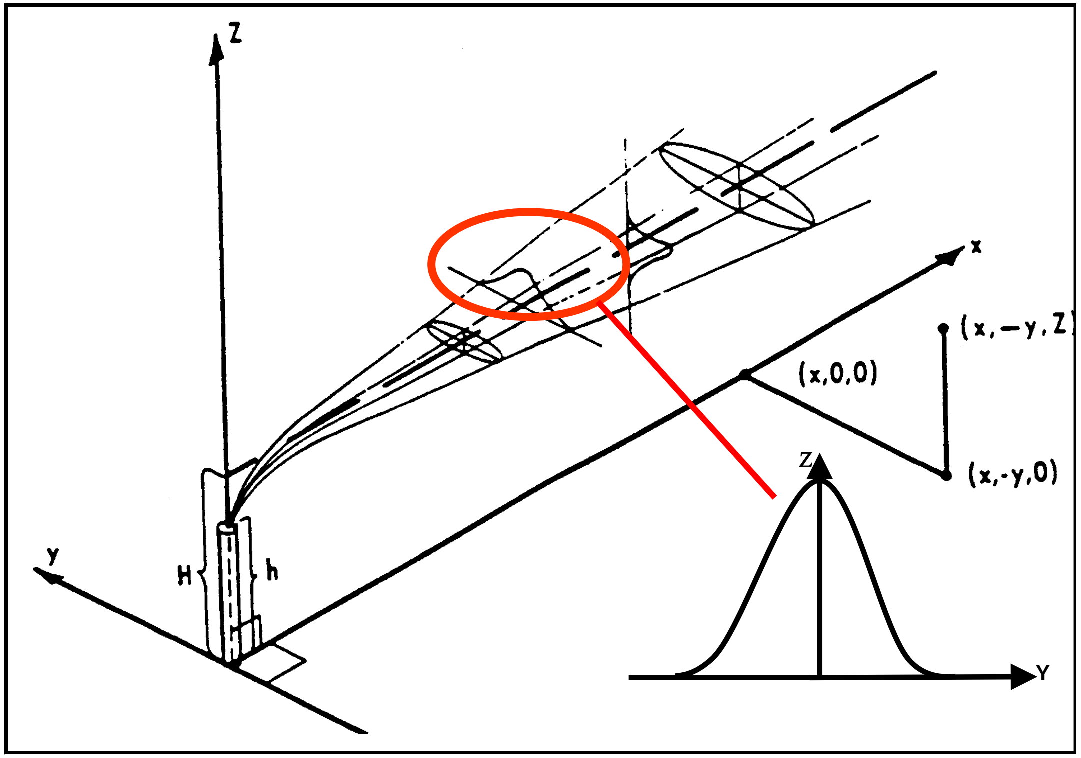
Validity: 1 cm < d < 10 km

E.g. Code_Saturne (EDF), Flacs (GEXCON), PANEPR (Fluidyn), FDS (NIST), Fluent (ANSYS)…



Gaussian models

Suitable for **passive dispersion**: pollutant transported by the wind and diffused by atmospheric turbulence alone



- Concentration calculated along plume axis
- A Gaussian (statistical) law is used to determine the concentration in the whole plume
- Based on standard deviations σ_y, σ_z characteristic of atmospheric turbulence, according to the **stability class,** environment…

$$C(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{(y-y_0)^2}{2\sigma_y^2}\right)\left[\exp\left(-\frac{(z-z_0)^2}{2\sigma_z^2}\right) + \alpha \exp\left(-\frac{(z+z_0)^2}{2\sigma_z^2}\right)\right]$$

"Integral" tools

Suitable for dispersions such as jet, heavy gas, light gas or passive dispersion

Tools of intermediate complexity

- Often contain a release source calculation module
- Integrate different models (jet model, dense gas, light gas…)
- Gaussian model used for the final (passive) dispersion phase

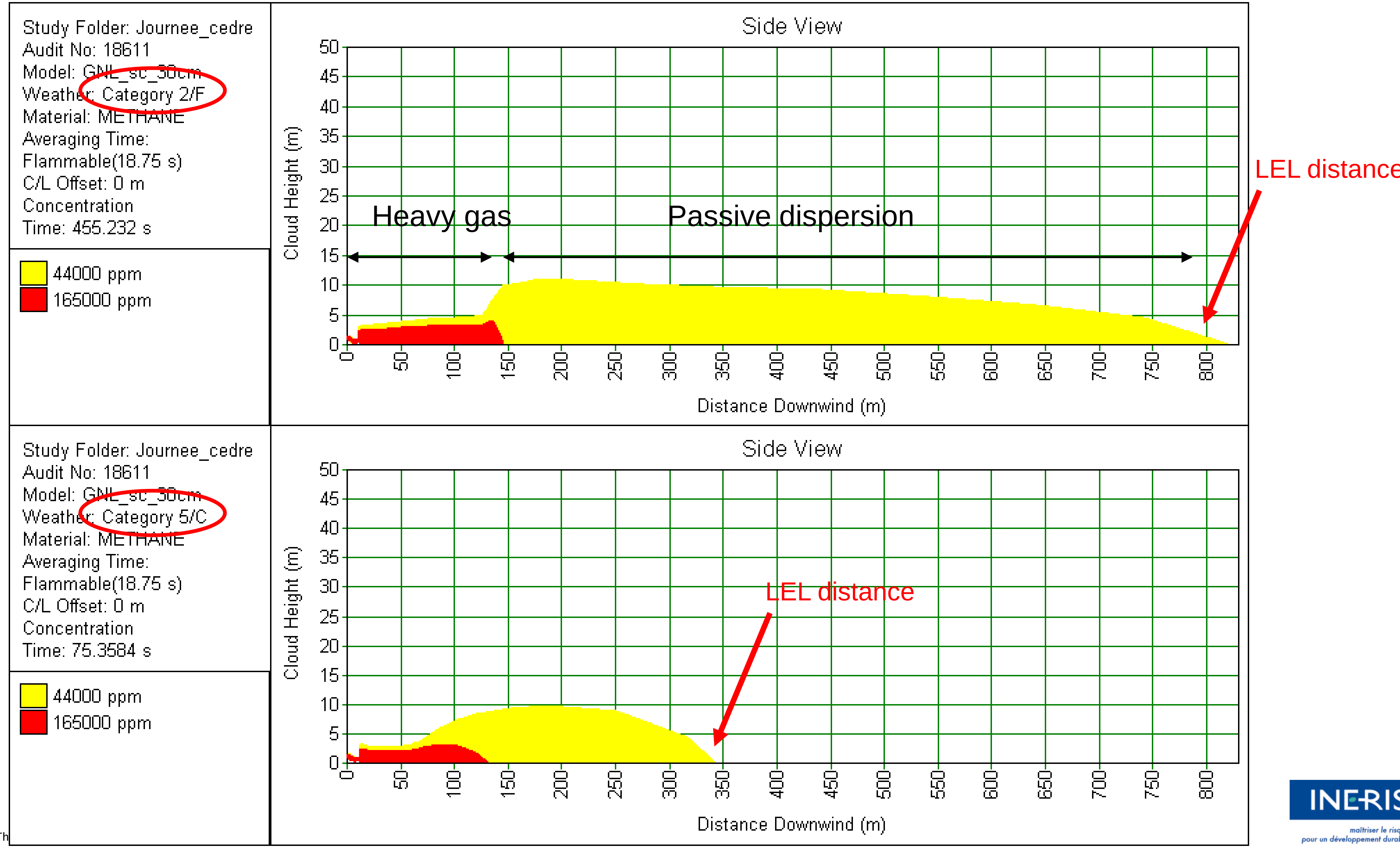
Similar advantages to those of Gaussian models

- Consideration of inversion layer
- Good validation on flat ground

Limitations (similar to Gaussian models)

- Constant weather conditions, flat ground (no relief or obstacles)
- Fairly unsuitable for low wind conditions (molecular diffusion not considered)

"Integral" tools: example

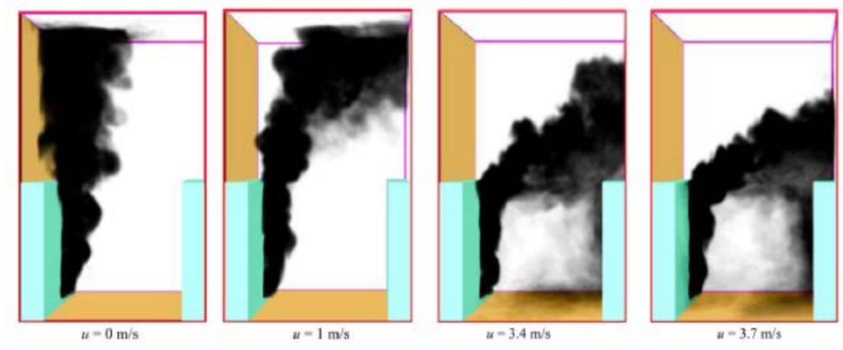


"CFD" tools (Computational Fluid Dynamics)

Specific advantages

- Explicit consideration of obstacles
- Explicit consideration of relief

⇒ Simulation **of complex environments**



Source : Documentation code FDS

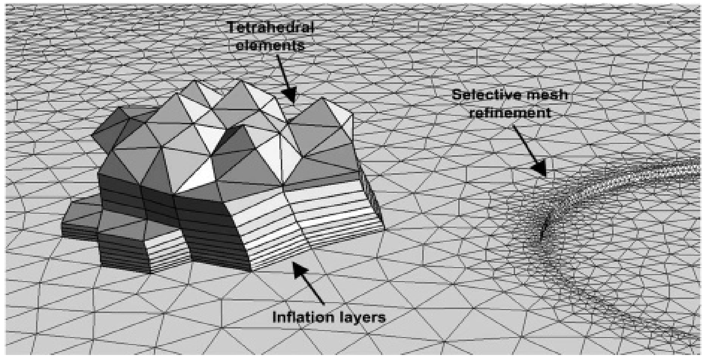
Several "sub-types"

- Eulerian (flow)-Lagrangian (dispersion)
- Eulerian-Eulerian
- Turbulence models: RANS (k-ε, …), LES, DNS

Limitations

- Numerous numerical parameters and input data
- Long calculation time
- Accuracy depends on resolution method, mesh used, boundary conditions, choice of turbulence models…

→ Costly



Example of complex meshing (Sklavounos & Rigas, 2006)

⚠ high variability of atmospheric dispersion results

> Beware of a safety approach by prediction!

Validation of atmospheric dispersion calculation tools?

Statistical criteria for validation by comparison with trials

$$FB = \frac{(\bar{C}_o - \bar{C}_p)}{0.5(\bar{C}_o + \bar{C}_p)},$$

$$MG = \exp\left(\overline{\ln C_o} - \overline{\ln C_p}\right),$$

$$NMSE = \frac{\overline{(C_o - C_p)^2}}{\bar{C}_o \bar{C}_p},$$

$$VG = \exp\left[\overline{(\ln C_o - \ln C_p)^2}\right],$$

$$FAC2 = \text{fraction of data that satisfy } 0.5 \leqslant \frac{C_p}{C_o} \leqslant 2.0$$

(Hanna and Chang , 2004)

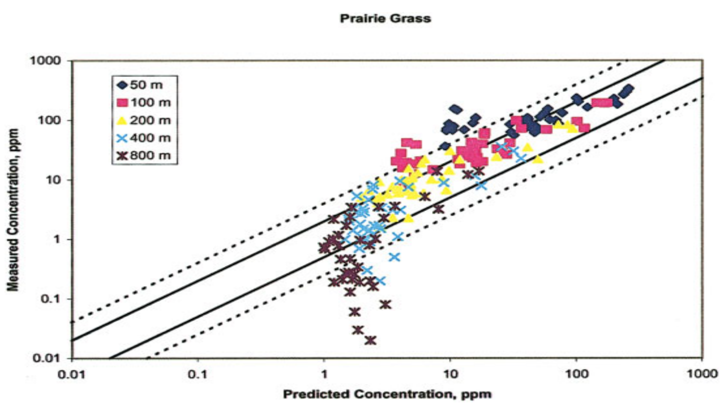
When a model is ideal...

FB = NMSE = 0
MG = VG = 1
FAC2 = 100%

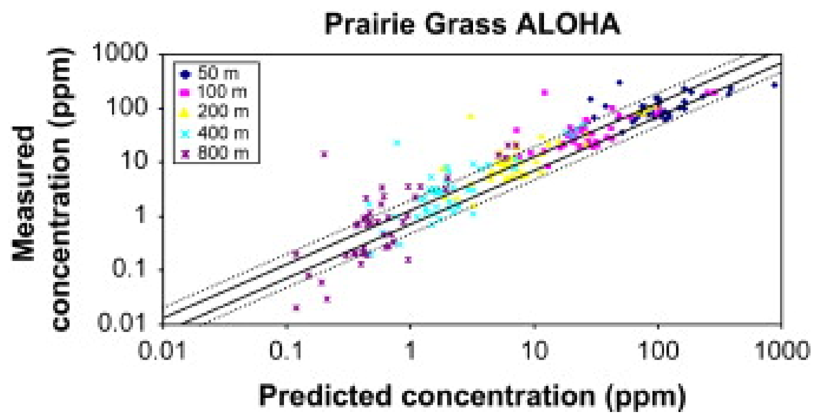
When a model is "good"...

-0.3	<	FB	< 0.3
0.7	<	MG	< 1.3
		NMSE	< 0.5
		VG	< 1.6
0.5	<	FAC2	

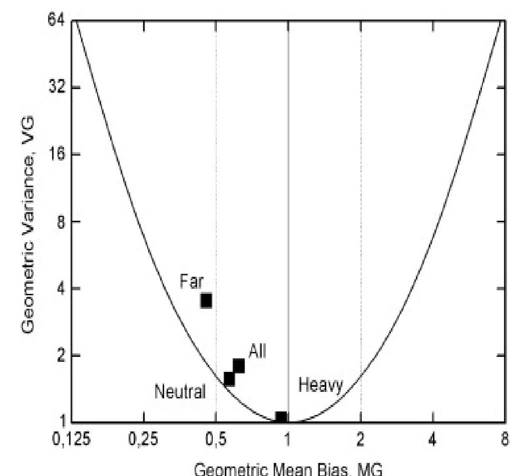
C_p: predictions
C_o: observations



(Dharmavaram et al., 2005)



(Mazzoldi, 2008)



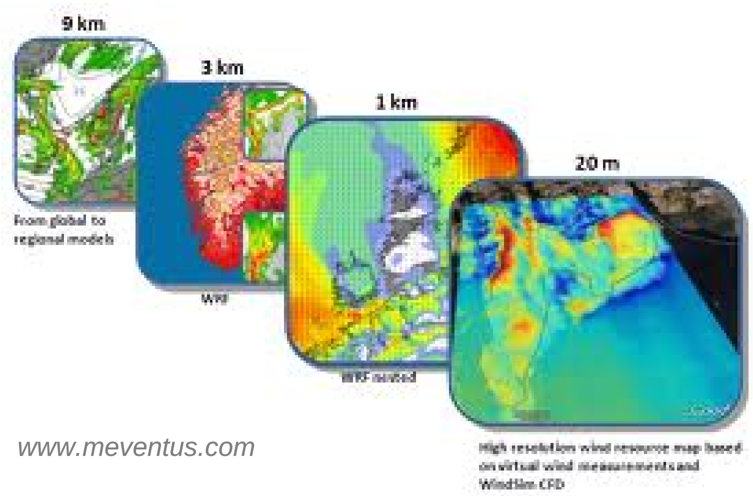
(Kisa and Jelemensky, 2009)

Towards far-field dispersion…

Modelling far-field aerial dispersion (> a few km)

- Spatio-temporal evolution of weather conditions
- Relief, surface heterogeneity
- Eulerian, Lagrangian or mixed approaches
- Many models, often devoted to the simulation of chronic emissions and air quality (on large scale: Saharan dust, radionuclides, volcanoes…)

  ⇒ Possible <u>coupling</u> of local < regional < global scales



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