Added value and limitations of CFD codes within the framework of industrial safety: the specific case of atmospheric dispersion

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Industrial risks mastering in France

2001, September the 21st: Major explosion in Toulouse (AZF)

- 31 deaths
- 2500 injuries

Consequences: Modification of the industrial risk prevention strategy

2005: A new legal tool in France for protection people from industrial hazards

- PPRT (“Plan de Prévention des Risques Technologiques”)
- Requirement: Prediction of dangerous area in case of accident
- Consequences: financial and human impact: protection measures to expropriation
- Importance in computing precise distance to prevent people from exposure AND realistic safety cost

Dangerous phenomena and current approach

3 types of phenomena

- Fire
  - Radiation models
  - Integral and Gaussian approaches for smoke dispersion
- Toxic dispersion
  - Integral and Gaussian approaches
- Explosion
  - Integral and Gaussian approaches for vapour dispersion
  - Analytical models enriched with experimental data

➔ A financial interest for explosion (glassbreak) and dispersion (large distance)

➔ Atmospheric dispersion appears as a key issue for effect prediction

Limits of current modelling approaches

Current approaches : Integral and Gaussian models

- \+ Design on experimental campaigns with free releases
- \+ Directly linked with atmospheric stability
- – Not able to take obstacles into account
- – Not able to predict kinetic aspects

A real requirement

➔ being more predictive in terms of distance for the different effects

Are other possibilities available?

Is CFD an improvement ?

Theoretically

CFD modelling ⇔ Fluid mechanics equation solving

➔ All physical phenomena must be taken into account

But, a significant dependance on

- Suitable boundary conditions in relation with wind stability
- CFD sub models to reproduce physical phenomena (thermal gradient effect, turbulence equilibrium, ...)

A finding : Different chosen approaches by user induce large variety in the computed distances

The French National Working Group

The objective

- To propose best practices in order to homogenise practises regarding atmospheric dispersion modelling with CFD

Three subgroups with specific thematic:

- Scientist WG: Physical models, visualisation and results interpretation, …
- Modelling WG: Simulations of blind fictitious cases, comparison with experimental results, parametric tests based on a dozen of users…
- Diffusion and communication WG: Application fields, results presentation and communication, …

Construction of best practices based on the computation of 2 blind tests

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First case: Free land atmospheric dispersion

3 different toxic gas releases of several kg/s mass flow rate under high pressure through 2 inches hole

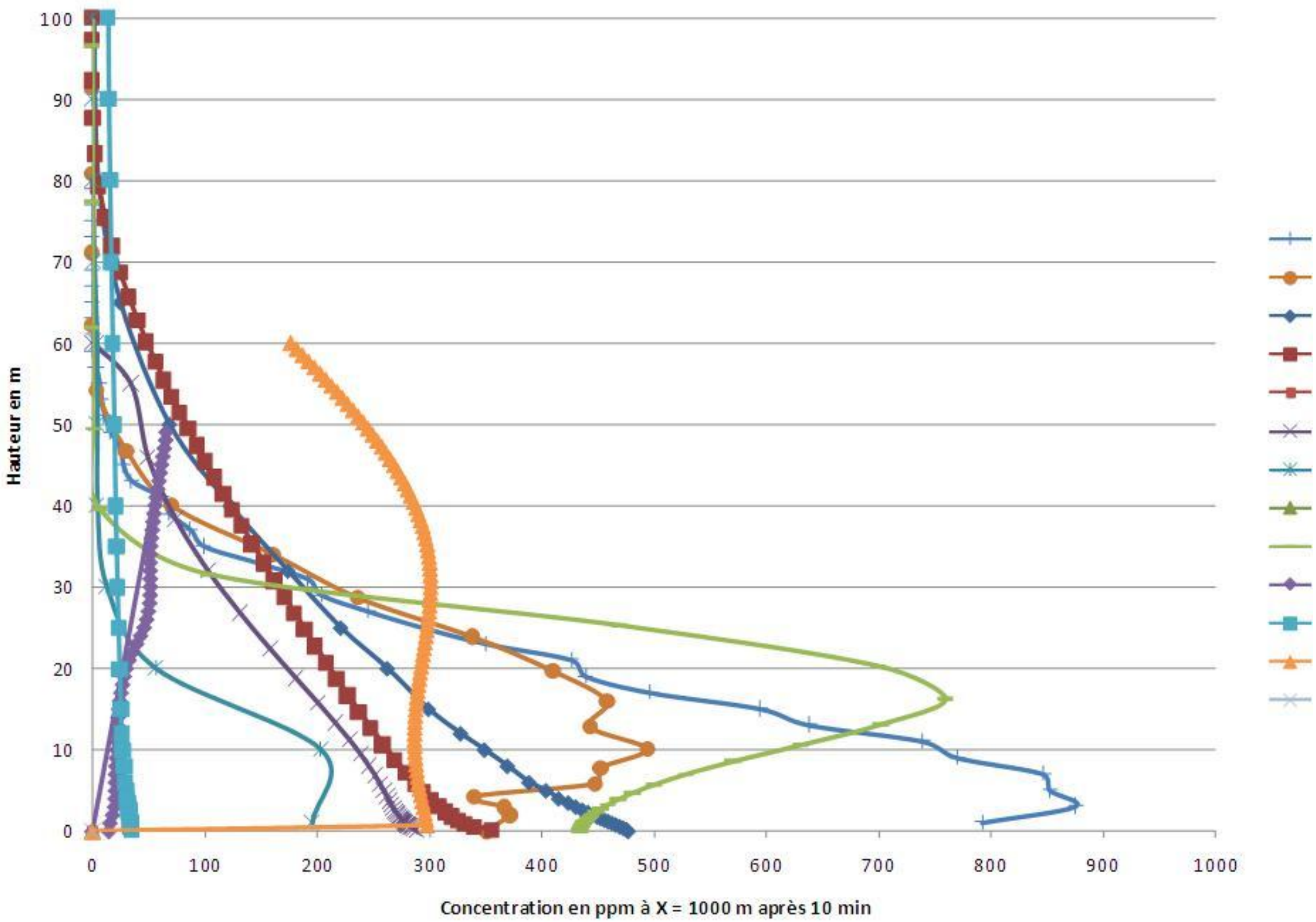
- Heavy
- Neutral
- Light

2 different wind profiles

- Stable: F3
- Neutral: D5

Users are fully free: no constrain on wind representation, turbulence modelling, boundary conditions, source term, etc

Results for case 1: Vertical concentration profiles



Learning from case 1

Unacceptable discrepancy in the results

Choice of the models is specific to each user

4 major items of choice were identified:

- **Interpretation of wind profile as input for CFD**
- Turbulence models
- Mesh : cells size
- Source term implementation

Need to harmonize the methodology for these 4 items as far as possible

Relation between wind profiles and CFD approach

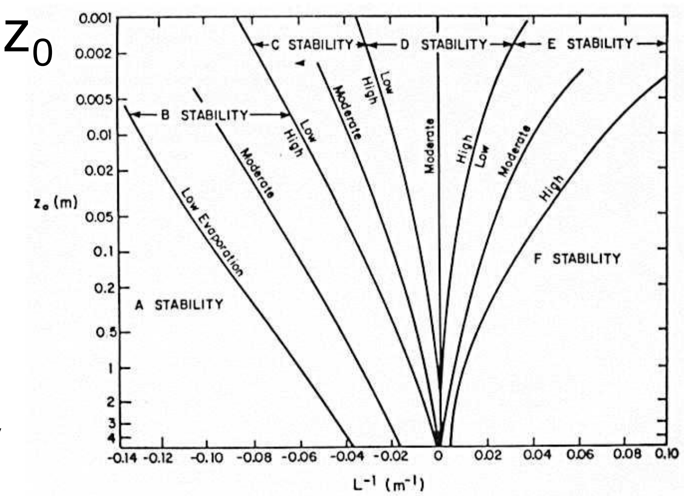
French regulation requires atmospheric conditions as F3 or D5

- But these conditions cannot be introduced easily
- For a condition, several profiles are possible

No interpretation rule exists to build profile for CFD models

- 3 parameters are used as inputs: U_{ref}, LMO et z_0
- Relation of wind class and LMO/z_0 within Golder approach

➔ Surface boundary layer profile



- Extension above surface layer: Gryning theory

Great work in order to establish a consensus on these parameters

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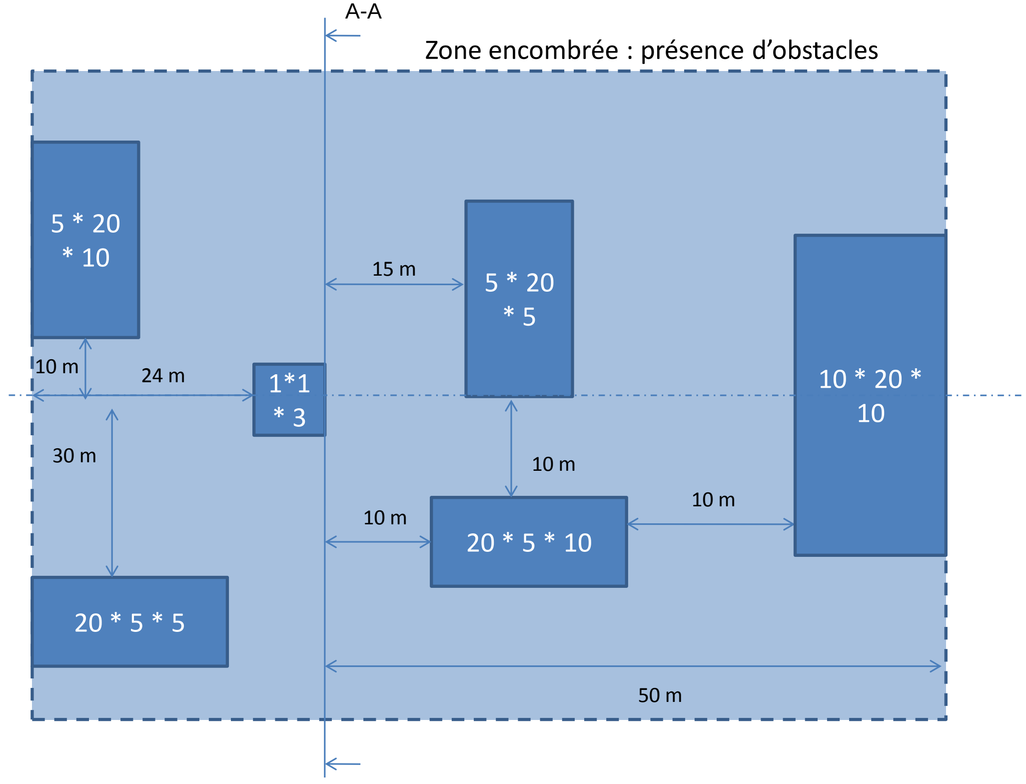
Second configuration: modelling with obstacles

Some parameters were fixed:

- Wind profiles
- Simpler source term

Obstacles were introduced inside the domain

About 12 modellers



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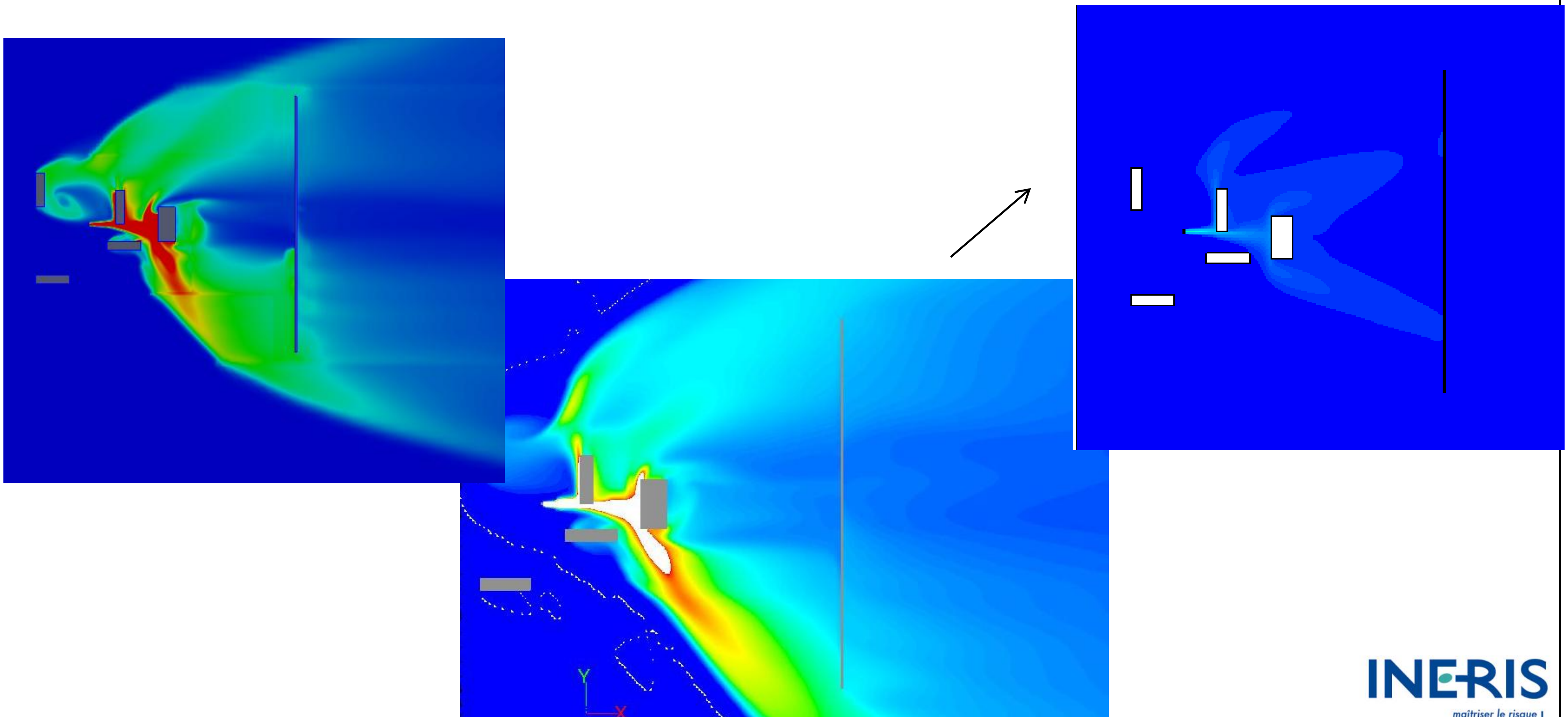
Second case: Overview of the results

Differences still observed

Differences between different users of a same code



Turbulence modelling

Two main approaches

- Averaged approach: RANS, mainly k-ε
- Large scale turbulence modelling: LES

For similar turbulence models (k-ε), most influencing parameters are

- Buoyancy effects
- Surface or volume source term
- Mesh
- Building roughness modelling

Specific work on this topic

- Consideration of turbulence production by buoyancy effects
- Numerical domain must be extended enough upstream first obstacles

Production of a list of best practices (I)

- The need of a user calibrated code
  - Beyond the validity of the code, user must be aware
  - CFD using requires physical sense for downstream analyse
- Boundary conditions position
  - Necessity of a distance upstream first obstacle
  - Distance of the domain roof
- A consistent mesh
  - Mesh independence
- The use of non dissipative numerical schemes
  - Numerical diffusion ➔ artificial reduction of dangerous area

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Production of a list of best practices (II)

- Proposition of wind profiles that correspond to Pasquill classification
  - Possibility to be in accordance with regulation
  - Consistent with the concept of prediction
- Wind profile conservation along the domain
  - Atmospheric turbulence has to be maintained
  - The criteria: F3 at the inlet ➔ F3 at the outlet
- Use of a turbulence model that enables taking into account atmospheric phenomena
  - Necessity of taking into account the production term due to buoyancy effects

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Atmospheric dispersion modelling tools

What about commonly used models

- Same homogenization to be done for semi-analytical models
- How is modelled wind profile ?
- Is it relevant to model dispersion along cliff with semi-analytical model?

CFD added value

- Definition of wind profile
- Reflection on turbulence modelling

Conclusions

On CFD use for industrial safety

- Not an improvement for simple case
- Appears as a very relevant way for complex cases considering best practices can effectively be enforced
- What is a complex case?

➔ Requires a high level of physical knowledge for the user

Perspectives

Regarding WG

- Experimental comparison
- Kit Fox Field with continuous release (180 s)
- Simulations with the proposed **best practices**
- Still some differences but ... Is it worth than other models ?