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V Convegno Nazionale

Il controllo degli agenti fisici: ambiente, salute e qualità della vita

Novara, 6 giugno 2012

ESSEM COST ACTION ES1006. Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments.

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COST is supported by the EU RTD Framework Programme

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COST is an intergovernmental framework for European Cooperation in Science and Technology, allowing the coordination of nationally-funded research on a European level.

- supports capacity building by connecting scientific communities
- provides networking opportunities
- connecting research with stakeholders

ESSEM Domain:

Earth System Science and Environmental Management

ESSEM encompasses the rapidly-growing science and technology agendas relating to better understanding, observing, modelling and predicting the Earth system and thereby improved management of environmental conditions.

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Why COST ES1006 …

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- different communities/bodies deal differently with similar problems of hazmat dispersion at local scales

  → establish a dedicated, non-competitive platform for information exchange

- numerous research and development activities at national level

  → create a cross-community network necessary for further building of capacity

- end users / stakeholders often not fully aware of limitations and restrictions of existing tools

  → characterize, quantify and verbalize advantages and limitations of model approaches

- end users / stakeholders often not aware of advanced capabilities in local-scale airborne hazards modelling

  → promote improvement of local-scale hazmat dispersion modeling

COST ES1006 deliverables

- establishing consensus on the 'state-of-the-art' in local scale airborne hazards modelling
- providing common means, tools and data for rigorously testing and evaluating models
- providing guidance for reliable use of models in the context of local-scale emergency response
- developing and testing strategies and methodologies for new advanced modelling approaches
- **bringing together scientists and emergency planning&response specialists**

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http://www.cost.eu/domains_actions/essem/Actions/ES1006

The motivation

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Accidental or deliberate releases of hazardous materials in populated areas induce a growing concern in the society.

Instantaneous accidental releases from ………

Industrial sites

Energy facilities

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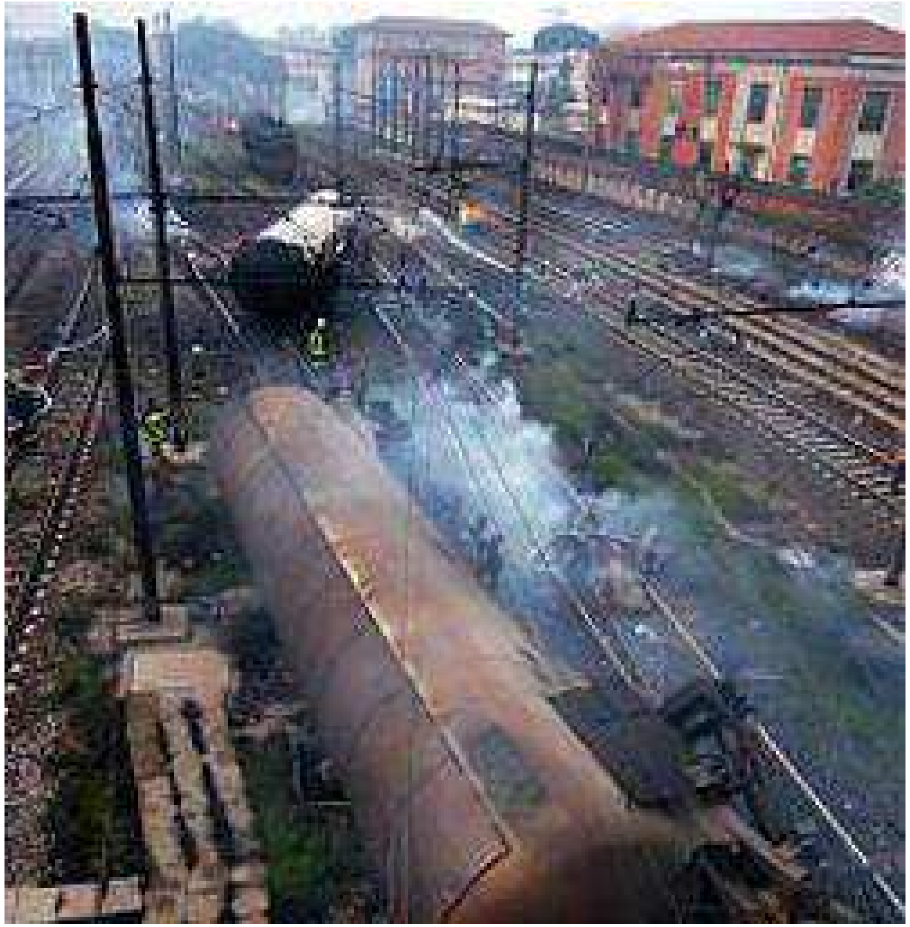
Transportation of hazardous materials



Terrorist attacks

Accidental or deliberate releases of hazardous materials in populated areas induce a growing concern in the society

Instantaneous accidental releases from….

- industrial sites,
- energy facilities,
- transportation of hazardous materials
- or even a CBRN (Chemical-Biological-Radiological-Nuclear) terrorist attack

…. can lead to catastrophic consequences in terms of population casualties and damage to ecosystems and infrastructures.

Dealing with such releases is complicated by the need for a fast and at the same time sufficiently accurate emergency response tool.

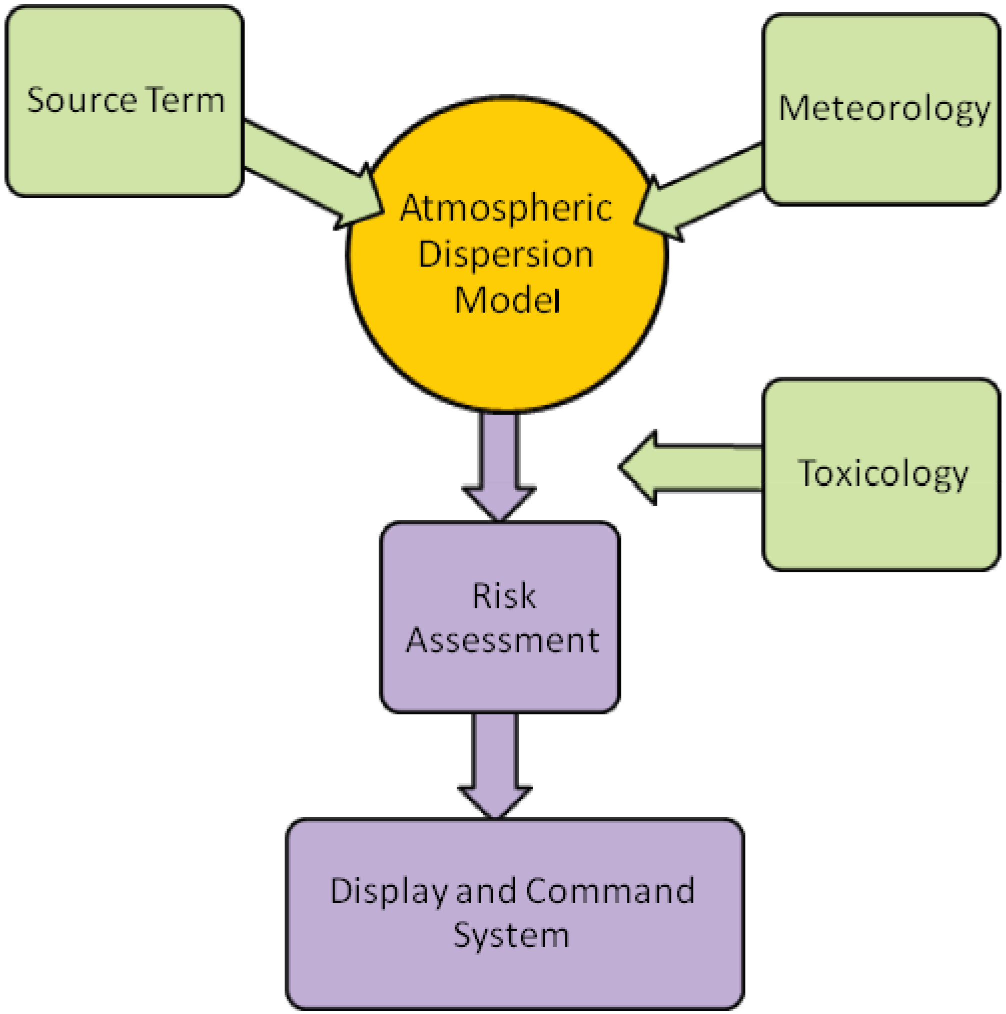
The Emergency Response Tools....

Emergency response tools take the form of fully integrated management systems, or modular concepts that have interfaces between the individual components.

They all have to provide the means to:

- Characterise potential hazards;
- Manage the logistical aspects of emergency incident response;
- Account for different types of release;
- Document the decisions and actions taken during an incident, to facilitate comprehensive post-incident analysis.

Substantial progress in computational and information technology led to the development of sophisticated emergency response management systems.


Source Term
Meteorology
Atmospheric Dispersion Model
Toxicology
Risk Assessment
Display and Command System

… and the dispersion models

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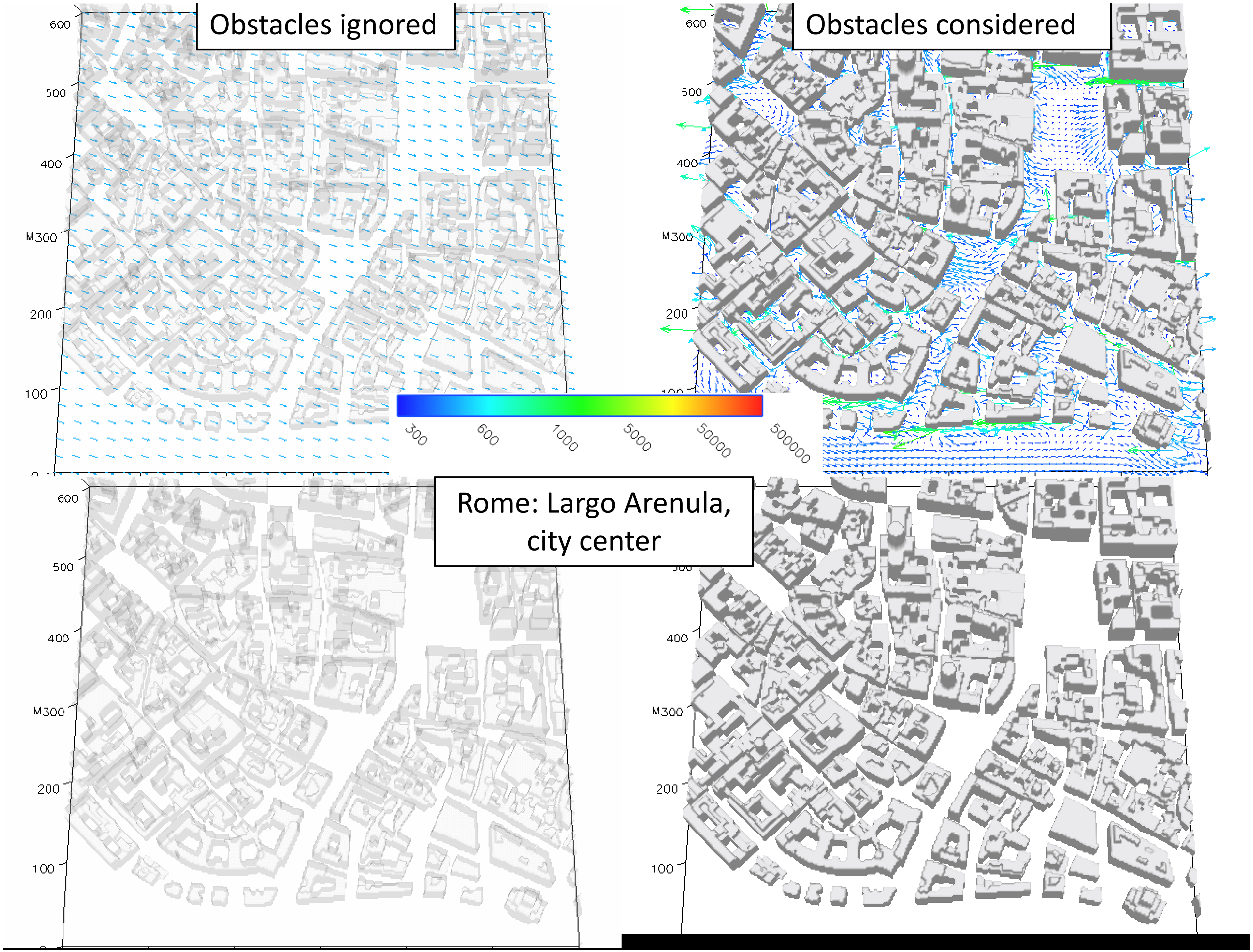
A crucial part of a state-of-the-art emergency response management tool is represented by the **airborne hazards dispersion models** : *these, combined with sensors that detect and measure hazardous material concentrations are the backbone for any comprehensive emergency management system*.

One of the biggest scientific challenges in local-scale emergency response remains the prediction of airborne hazards dispersion from accidental or deliberate releases at the very local scale, especially within complex environments.

If dispersion of agents and resulting threats are unknown, all subsequent steps of modern emergency response and management quickly become questionable, inefficient and maybe even threatening for first responders.


Obstacles ignored
Obstacles considered
Rome: Largo Arenula, city center
300
600
1000
5000
50000
500000
600
500
400
M300
200
100

Accidental, local scale, built environments...

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Due to its unexpected nature, an **accidental release** is a complex phenomenon and a challenging situation to handle.

First responders have to deal with a **highly problematic scenario** unfolding in an uncertain frame.

At the **local scale**, the situation is typically complicated by the following factors.............

Accidental, local scale, built environments…

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- the duration of the release is often very short (minutes only at most);
- the emission characteristics of the source (amount and type of material released, for example) are only partially known (if at all);
- the local meteorological conditions driving the spread of the contaminant are not readily available at the desired level of accuracy, and are subject to constant change;
- the release occurs in a complex industrial or urban environment, where the release of even small amounts of hazardous material can instantly pose a severe threat to the surrounding population.
- the response time in which to mitigate the effects of a release is short (typically less than an hour);

The focus and aims in practice

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The **main focus** of COST Action ES1006 is to improve the quality and robustness of local-scale predictions of airborne hazard dispersion from accidental or deliberate releases in complex urban and industrial environments.

The Action **aims** at establishing a scientific and methodological reference for local-scale airborne hazard modelling through:

✓Improving the scientific basis behind local-scale dispersion modelling;

✓Developing an inventory of models and modelling systems;

✓Developing comprehensive practical guidance for using models to track and predict the dispersion of airborne hazards.

The tasks

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The **major tasks** of the Action are to :

➢ Review the current tools and models used in characterising hazard dispersion and examine how these are applied operationally in emergency response efforts…. **DONE!**

➢ Identify the deficiencies in tools and models that limit their effectiveness and operational use in emergency situations; **ongoing**

➢ Identify the critical input data that must be available to use the tools and models effectively; **ongoing**

➢ Identify ways to improve the accuracy of tools and models. **coming soon**

➢ Measure the quality of model results and identify ways to improve them, a task-specific validation procedure will be adopted. **coming soon** *This will be based on a structured set of local threat scenarios that have been defined by their requiring models to have certain capabilities.*

The boundaries

The bounds of the Action activity are short of the final evaluation of the health and environmental effects.
This field of research needs the expertise of epidemiologists, toxicologists, physicians and biologists and requires a much wider interdisciplinary context than the existing Action can provide.

Publicly available exposure indices, such as those defined by the European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC, http://www.ecetoc.org/) will be considered and applied in the Action within the limits of the information provided

The structure

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Working Group 1 - Threats, Models and Data Requirements - is characterizing and categorizing existing models as well as typical release scenarios.

Working Group 2 - Test, Evaluation and Further Development - is defining (blind) test scenarios, testing and assessing different modelling approaches and is working on scientific strategies for improving the implementation of corresponding tools.

Working Group 3 - Applicability, Implementation and Practical Guidance – is dealing with the practical constraints in the use of local-scale emergency response models.

Review of Current & Future Threats & Challenges

The Threats / The notion of “CBRN agents”

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The **agents** : hazardous materials transported and dispersed in the air with diverse potential deleterious effects on the environment and on the human health

Groups of agents sharing common features, but different in nature, characteristics, changes during the dispersion time, health consequences:

- ✓ **C**hemicals
- ✓ **B**iological entities like bacteria, virus, spores…
- ✓ **R**adioactive elements or radionuclides
- ✓ **N**uclear fissile or fusible elements

Moreover… “**E**-threat” / ‘‘**F**-threat” – Releases may be associated with violent explosions / fires which:

a) Have a significant influence on the initial phase of the atmospheric dispersion
b) May produce significant numbers of casualties, irrespective of any dispersal of agent

The Threats / The types of Releases

Releases are characterized by the physical state or phase of the emitted species, leading to two major groups: gases or airborne particles called "aerosols"

Major differences between releases are due to **how** they are initially emitted into the atmosphere:

- ✓ Passive releases
- ✓ Buoyant releases (due to density differences)
- ✓ Releases with initial momentum (typically, a jet)
- ✓ Flashing and / or evaporating releases
- ✓ Chemically reactive releases

In many real situations, releases are not (thermo)dynamically and / or chemically passive

Atmospheric dispersion is not simply the "passive" emission of substances in the air, but generally associated with many different and complex interacting processes

Continuum of relative probabilities and magnitudes of threats posed by the release of various hazardous materials

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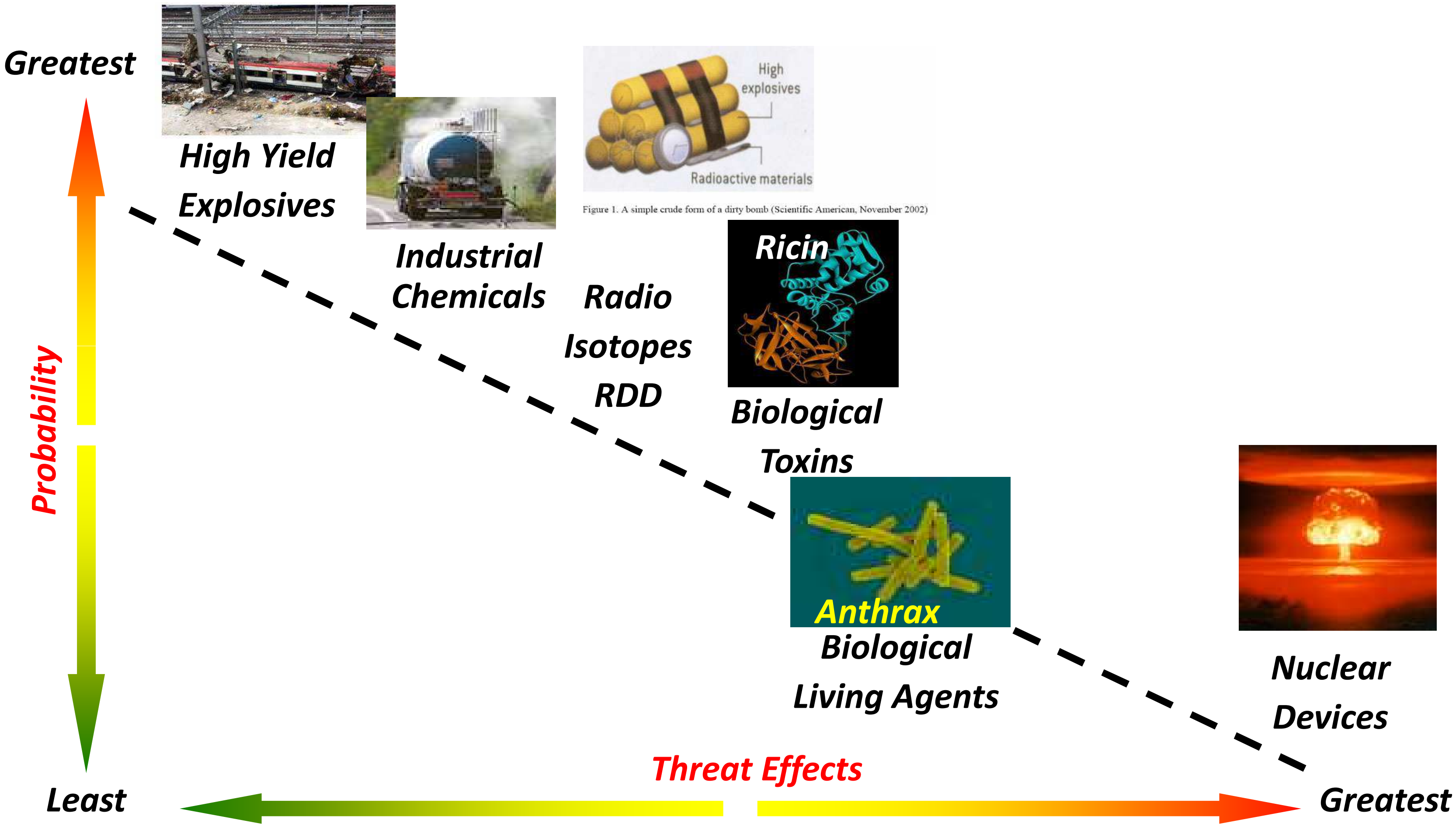

The challenges 1/4

The source term

✓To identify the location and typology
✓To estimate its geometry
✓To estimate the emission height (fixed or moving source?)
✓To identify the hazardous material
✓To correctly describe the initial conditions

The meteorological input

✓From measurements: they must be representative for the site where the release occurs and the plume of hazardous material disperses
✓From computations: must take into account the adapted level of detail for the site and scale of the modelling (e.g. effects of buildings)

The challenges 2/4

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The modelling

✓To account for complex built environments

✓To account for the specificity of the local scale (short-range) meteorology

✓To make the process efficient, i.e precise computations near the source and less refined calculations at some distance from it

✓To account for physical/chemical processes: *phase changes, aerosol genesis & evolution, chemical reactions, radioactive decay and formation of daughter products, degradation of biological agents*

✓To account for the dry or wet deposition of the hazmat – *at the ground, and any accessible surfaces (building roof and façades)* – and for their resuspension

The challenges 3/4

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The computational time

✓Must be acceptable but prescribes significant restrictions on atmospheric dispersion modelling and simulation techniques:

- *in preparedness phase, the time per case must be reasonable, but it is not the greatest concern*
- *in emergency phase, reliable results must be available very rapidly, with a compromise between precision and simulation duration*

✓Advances in High Power Computers and development of parallel versions of dispersion codes, is a critical factor in meeting the challenges in atmospheric dispersion

The challenges 4/4

The establishment of an operational tool

✓Has to be user-friendly for a broad range of users (*rescue services operator or dispersion expert*)

✓Has to include three essential modules: input data (*meteorology and source term*), dispersion computation, and consequences assessment

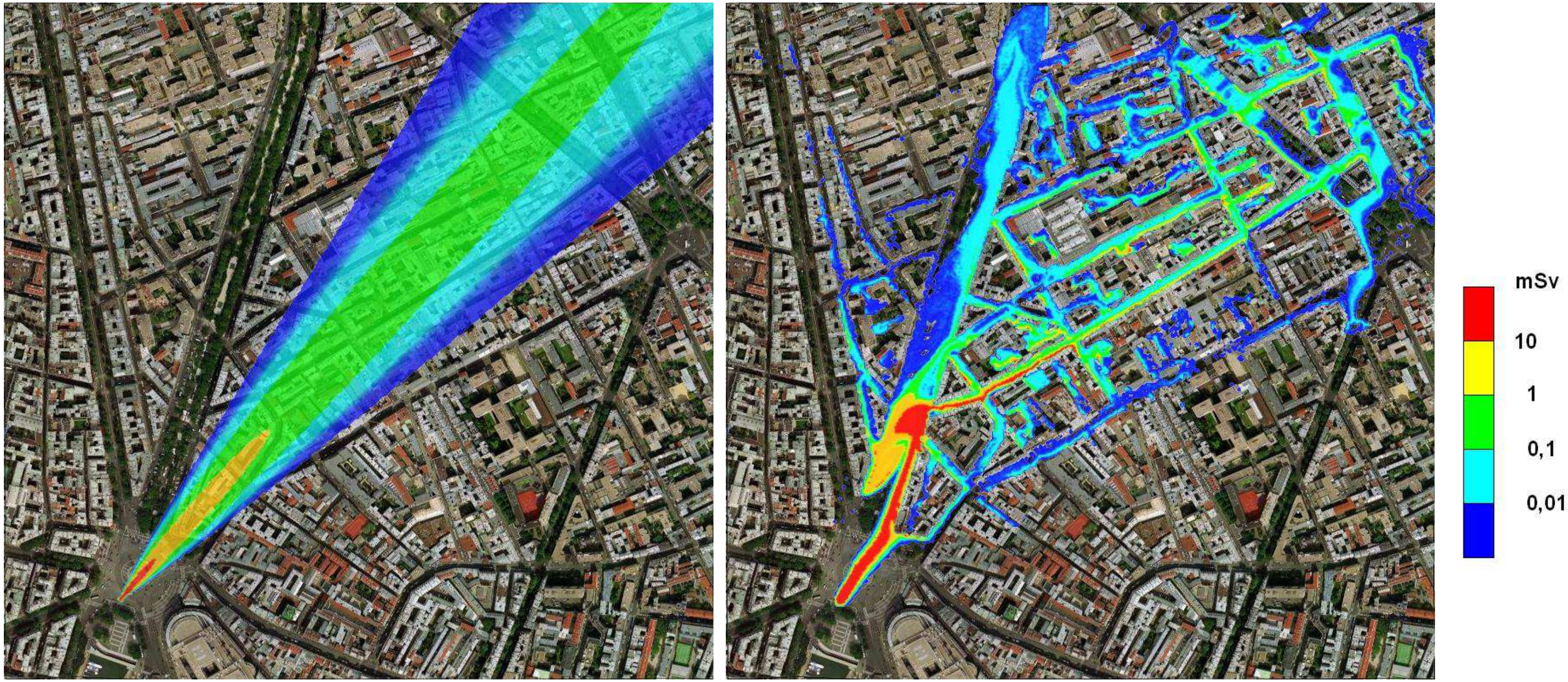
✓Has to be thoroughly verified and validated against experimental results

✓Has to be fully documented

- *Methods and equations in the reference manual*
- *Possible range of use and limitations of the code*
- *Implementation, computational detail and installation of the tool*
- *User guide presenting how to use the computational tool (full version and short version)*

✓Has to give a response in a time consistent with emergency situation providing quick and precise dispersion computations and output adapted to the needs of rescue teams and decision makers

An **open question** for the Action:
is it feasible to provide rescue teams and decision makers with (together!) a reliable, precise and quick answers Decision-Support System?



Total Effective Dose Equivalent (in mSv) resulting from the atmospheric dispersion of a radiological threat agent (3 TBq of ^{137}Cs) as seen by a simple Gaussian model and by a Lagrangian Particle Dispersion Model taking the buildings into account

N.B. As the LPDM uses a prediction of the local wind flow produced automatically and continuously, the dispersion and impact assessment results may be available within 5-15 minutes.

Review of Approaches and Tools

Concepts of TOOLS and MODELS

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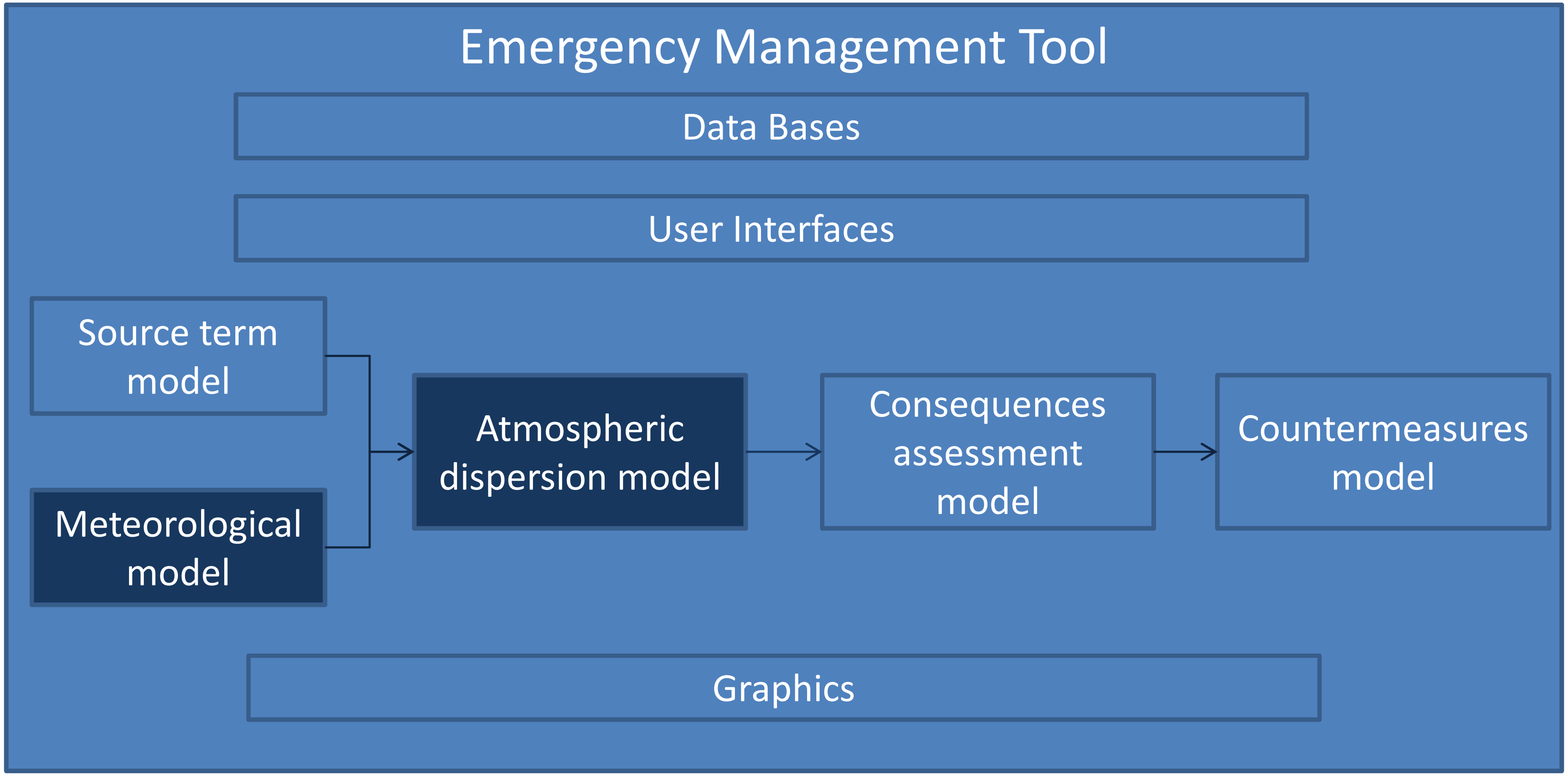
Tools: complete systems consisting of modules

Models: computational approaches or codes, components of “tools”



Concepts of SHORT-RANGE or LOCAL-SCALE modelling

Practice: “short range” includes distances from the immediate vicinity of the release up to a maximum radius of a few kilometres

“Short-range” (dispersion) ⇔ “Local-scale” or “Near-field” (flow)

Special emphasis in atmospheric dispersion of hazardous pollutants in urban environment:

- ✓Criticality (consequences, large numbers of people)
- ✓Complexity (mechanical and thermal forcing due to vertical buildings surfaces)

Active research in the direction of accurate and computationally fast approaches

Proposed classification for FLOW models

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A flow model calculates the flow conditions (wind vector, temperature, humidity, turbulence, solar radiation) over a given domain

- Classification by dimension
  - Uniform flow
  - Profile flow
  - 3-dimensional flow
- Classification by type of equations
  - 3-dimensional conservation equations of fluid mechanics ("prognostic")
  - Inter-(extra-)polation / (semi)empirical equations / mass-consistent wind flow models ("diagnostic")

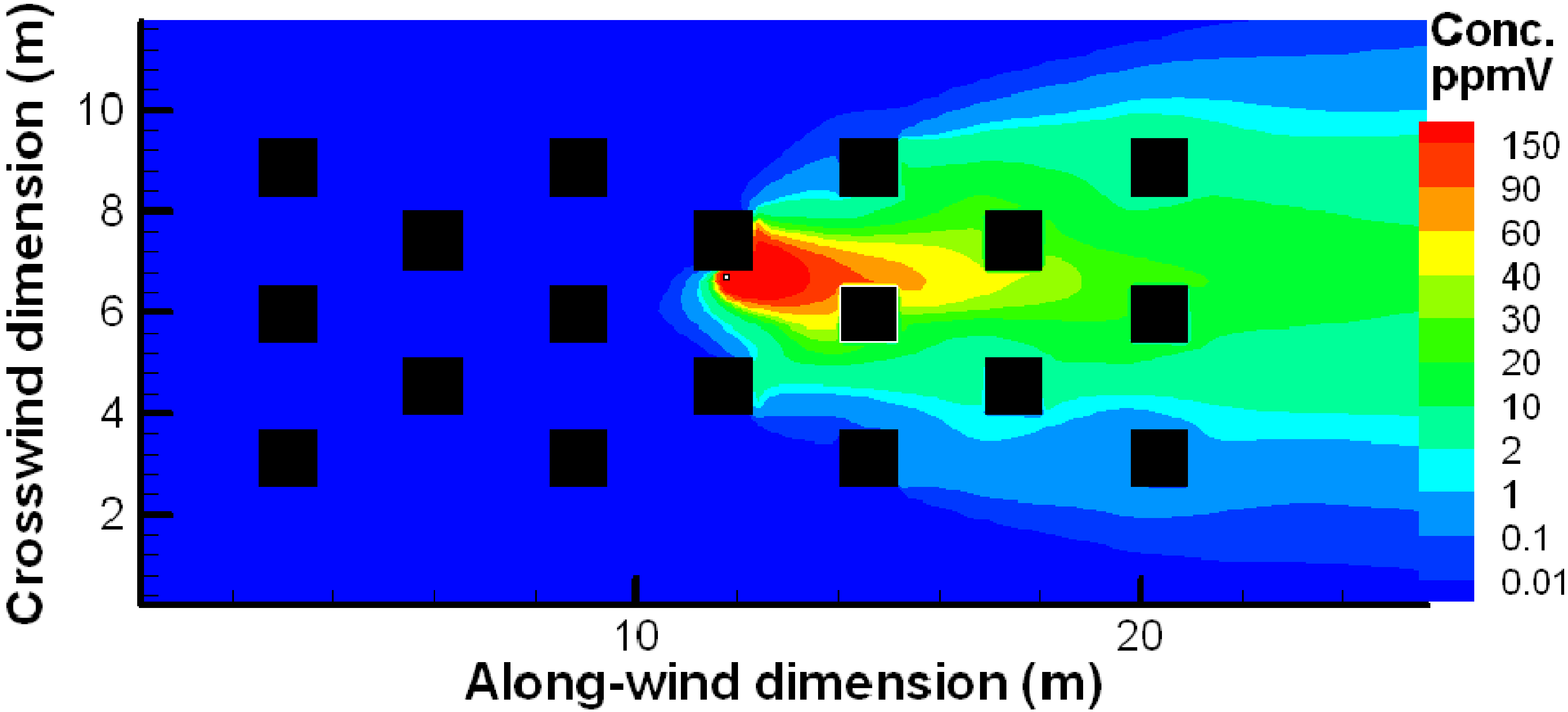
Proposed classification for DISPERSION models 1/3

- Frame of reference describing the dispersion process
  - *Eulerian*: solution of the conservation equation on a computational mesh in a fixed coordinate system
  - *Lagrangian*: movement of fluid parcels controlled by flow variables
- Types of conservation equations averaging:
  - *Ensemble* averaging: from a single “realisation” to the average of a large number of realisations
  - *Spatial* averaging: produces a coarser “grain” description of a dispersion realisation

Proposed classification for DISPERSION models 2/3

- Characteristic types of ensemble-average dispersion models:
  - Gaussian plume models: continuous releases, flat terrain, constant wind, Gaussian distribution of concentration
  - RANS (Reynolds-Averaged Navier-Stokes): numerical solution of conservation equations (momentum, species, energy) on a 3-D grid; parameterisation of turbulence; suitable for complex geometries; non-passive pollutants; high computational power required

- Characteristic type of spatially-averaged Eulerian model:
  - Large-Eddy-Simulation (LES): resolves largest turbulent eddies, parameterises sub-grid turbulence; very fine mesh required; high computational power required



Example of dispersion calculation by a RANS – CFD model

Proposed classification for DISPERSION models 3/3

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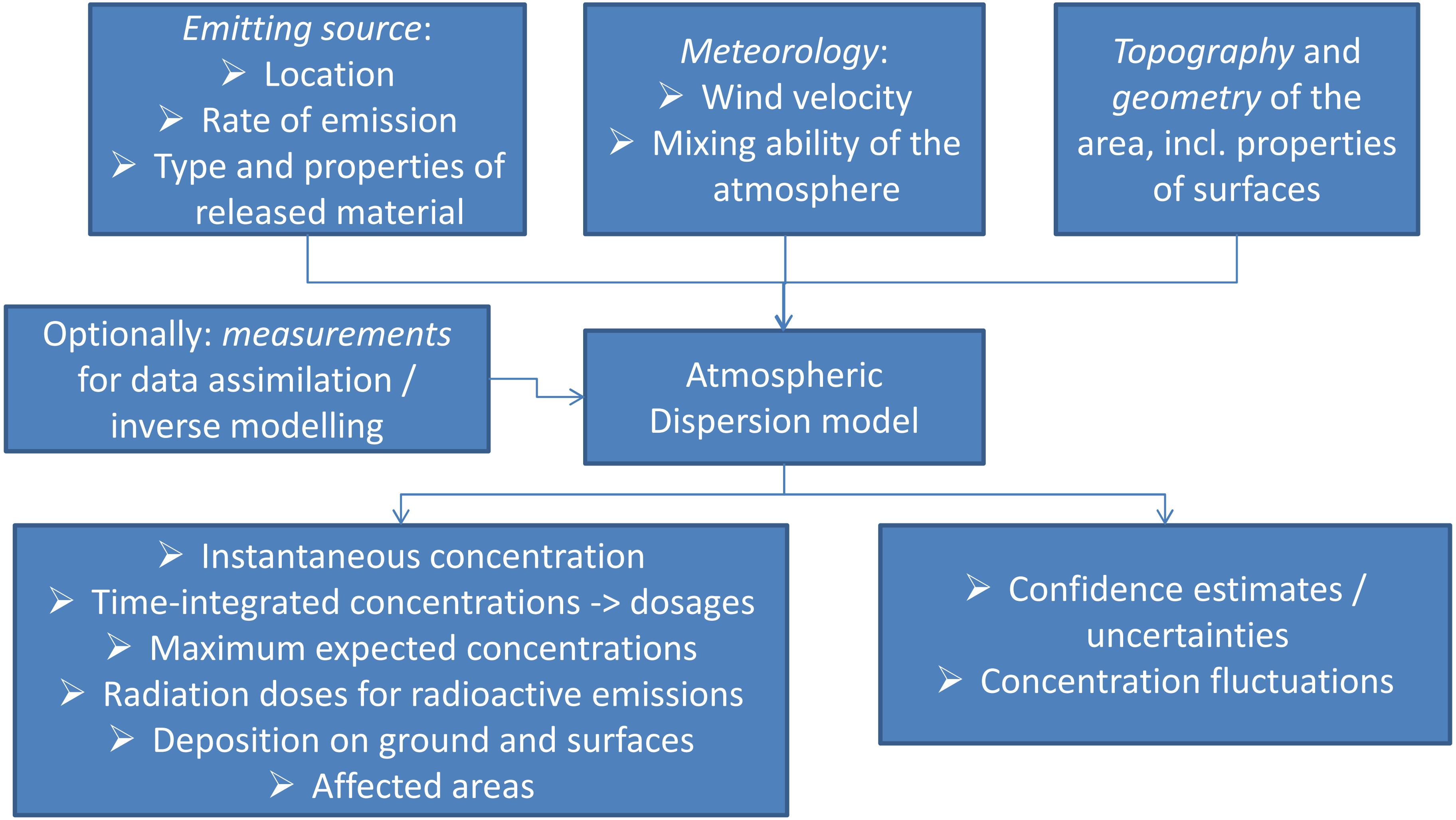
Lagrangian atmospheric dispersion models

- Puff: puffs transported with mean wind velocity, growing size with time, Gaussian distribution inside each puff, “kernel” method for concentration calculation
- Particle: Large number of virtual particles ($10^4 – 10^6$), mean wind velocity plus random motion (calculated by a stochastic equation, such as Langevin), concentration calculated by particles spatial density

- ✓ Realistic representation of dispersion, large number of particles required, so high computational power may be needed
- ✓ No “numerical” diffusion close to a point source, same details of dispersion at all scales
- ✓ Usually driven by prognostic or diagnostic wind flow models

Input and output requirements



Concepts of "When to use what" 1/5

Appropriateness of using a certain model type

- The time phase in relation to the emergency situation
- The spatial scales and other specific characteristics of the dispersion situation
- The availability of computational resources
- The reliability of the simulation results

It is customary to distinguish 3 phases in emergency management

- The preparedness phase
- The response phase
- The analysis and recovery phase

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The preparedness phase

- ✓ Contribution to the design / optimisation / enhancement of monitoring networks
- ✓ Risk assessments for defined threat scenarios
- ✓ Planning and training of personnel

- ➢ Computational speed of models not so important
- ➢ RANS-CFD / LES, Lagrangian particle models, wind tunnel studies

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The response phase

- ✓ Decision support for early responders
- ✓ If source is unknown: possible use of data assimilation and inverse modelling

- ➢ Computational speed of models very important (even compromising accuracy)

- ➢ First 1-2 hours: dispersion model with limited and basic input and short execution time

- ➢ Next several to 12 hours: more advanced model can be used

Concepts of “When to use what” 4/5

The recovery and analysis phase

- ✓ Contamination evolution at later stages
- ✓ Exposure assessment
- ✓ Assessment of need for responses and allocation of appropriate resources
- ✓ Identification of potential hot spots

➢ Accuracy of models predictions is more important here than computational speed.

➢ RANS-CFD / LES, Lagrangian particle models

Concepts of “When to use what” 5/5

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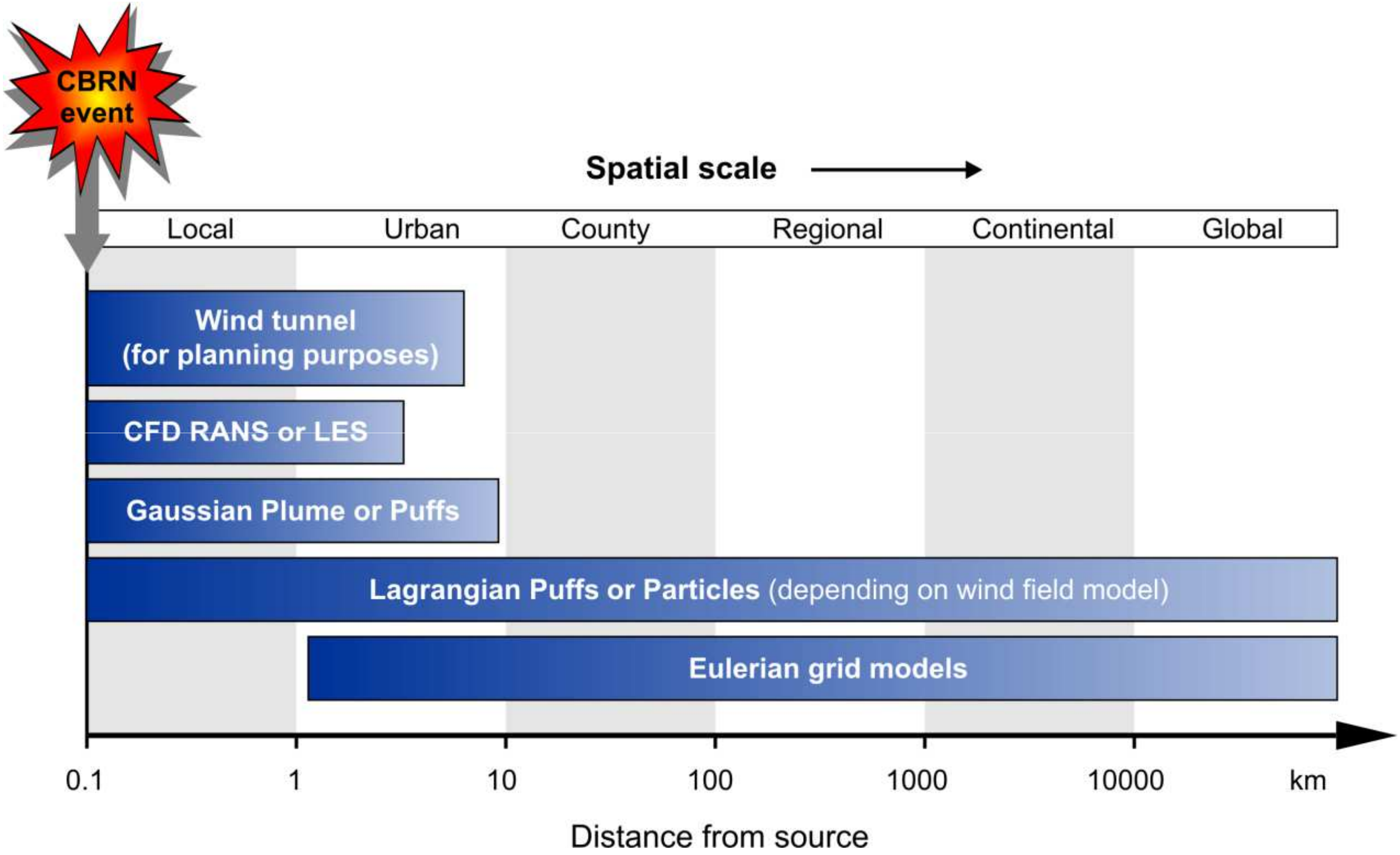

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Survey on Quality Assurance

Quality assurance in computational modelling

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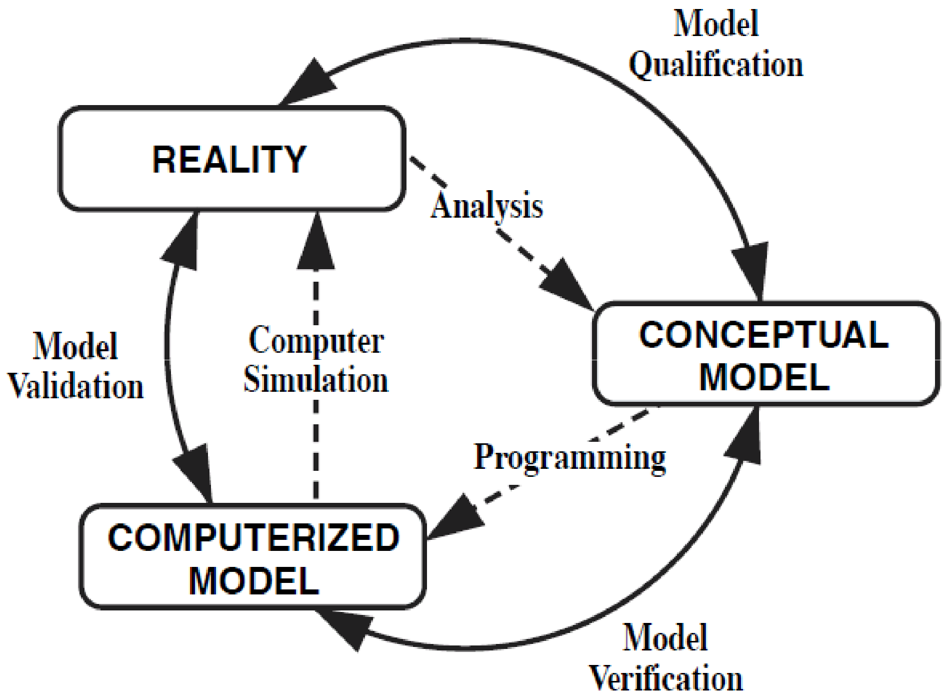
- Scientific review
- Assurance of correct coding (code verification)
- Comparison of model results with experimental data (validation)
- Uncertainty quantification for validation and prediction
- Operational evaluation



(Schlesinger, 1979)

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Verification: the process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model (AIAA, 1998).

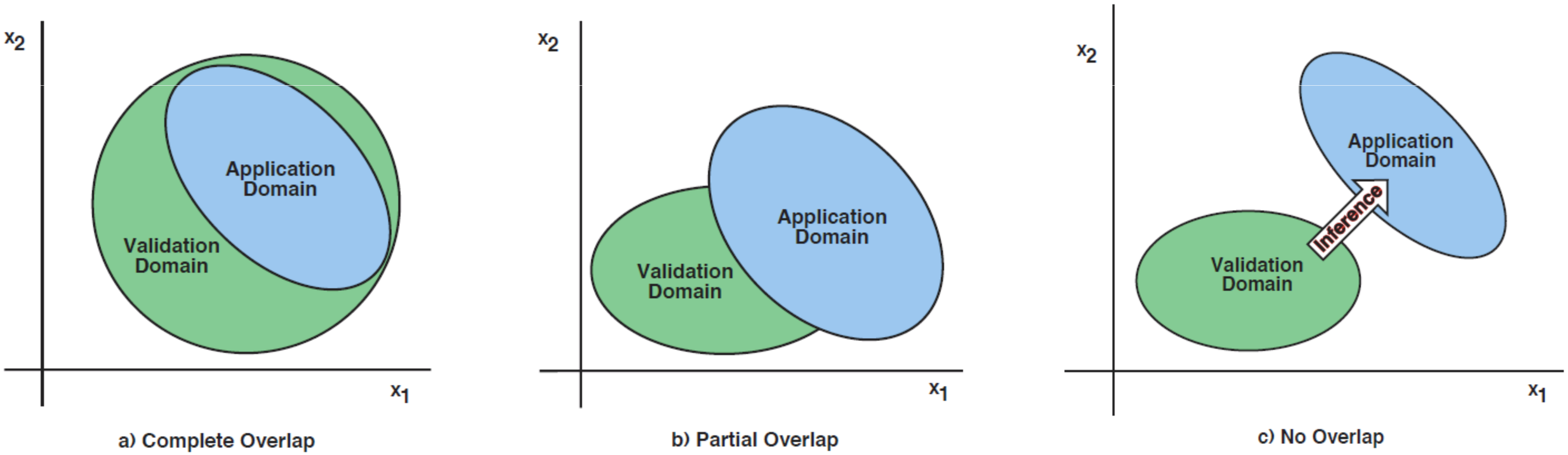
=> Mathematics: Are the equations solved right?

Validation: the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model (DoD, 1994).

=> Physics: Are the right equations solved?

Prediction

Prediction: use of a computational model to foretell the state of a physical system under conditions for which the computational model has not been validated (AIAA, 1998).



(Oberkampf et al., 2002)

Validation for hazmat dispersion modelling

Intended use: prediction of concentrations at local scale in complex built areas, which

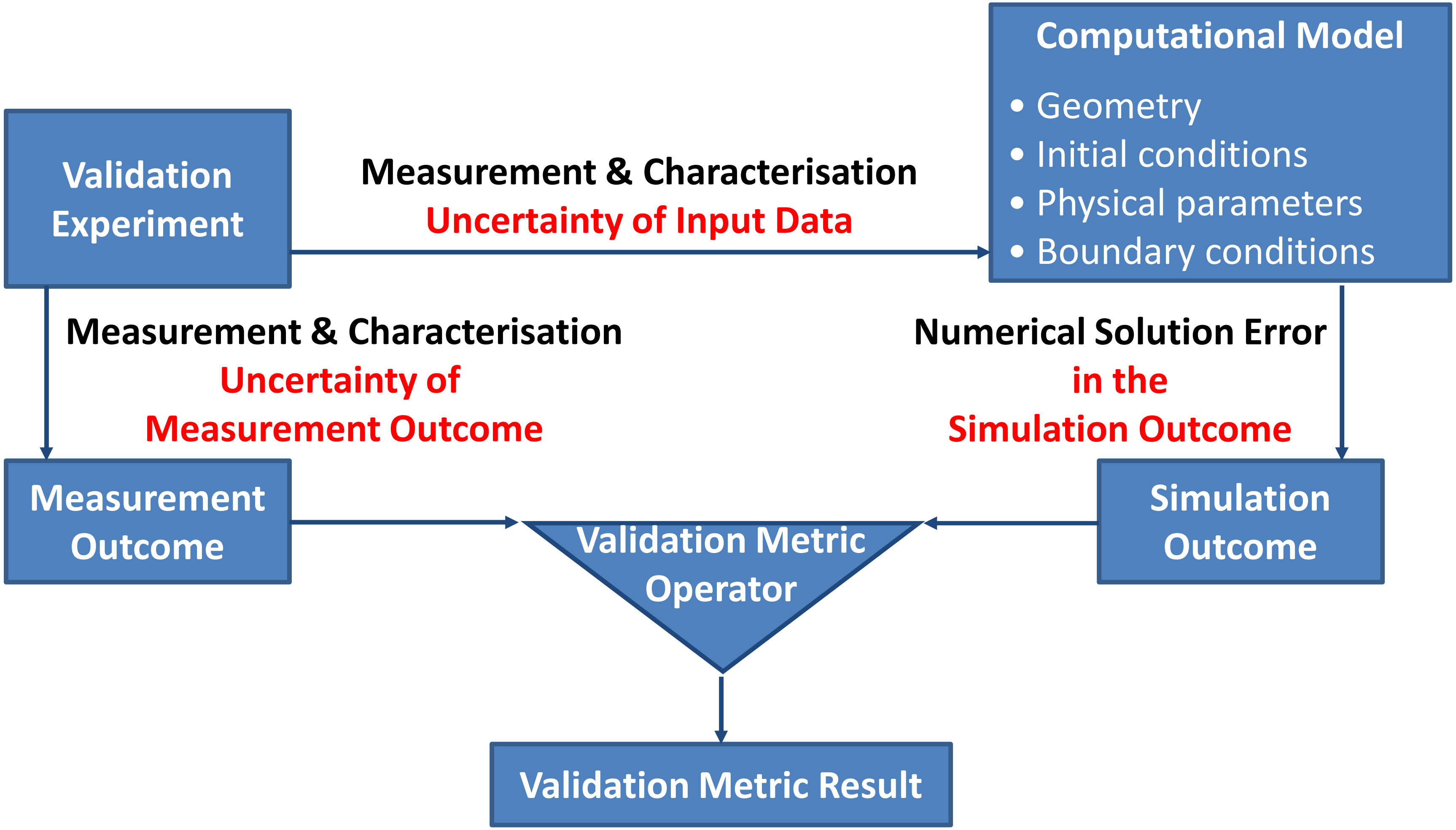
- are inhomogeneous in space and intermittent in time
- strongly depend on local wind field / meteorology

Accurate representation of the real world: comparison of model outcomes with experimental validation data, which

- are highly representative in space and time,
- have detailed information on external / initial conditions,
- are repeatable with known quality.

=> very demanding for field measurements!

Uncertainty quantification 1/3



adapted from Oberkampf and Roy (2010)

Uncertainty quantification 2/3

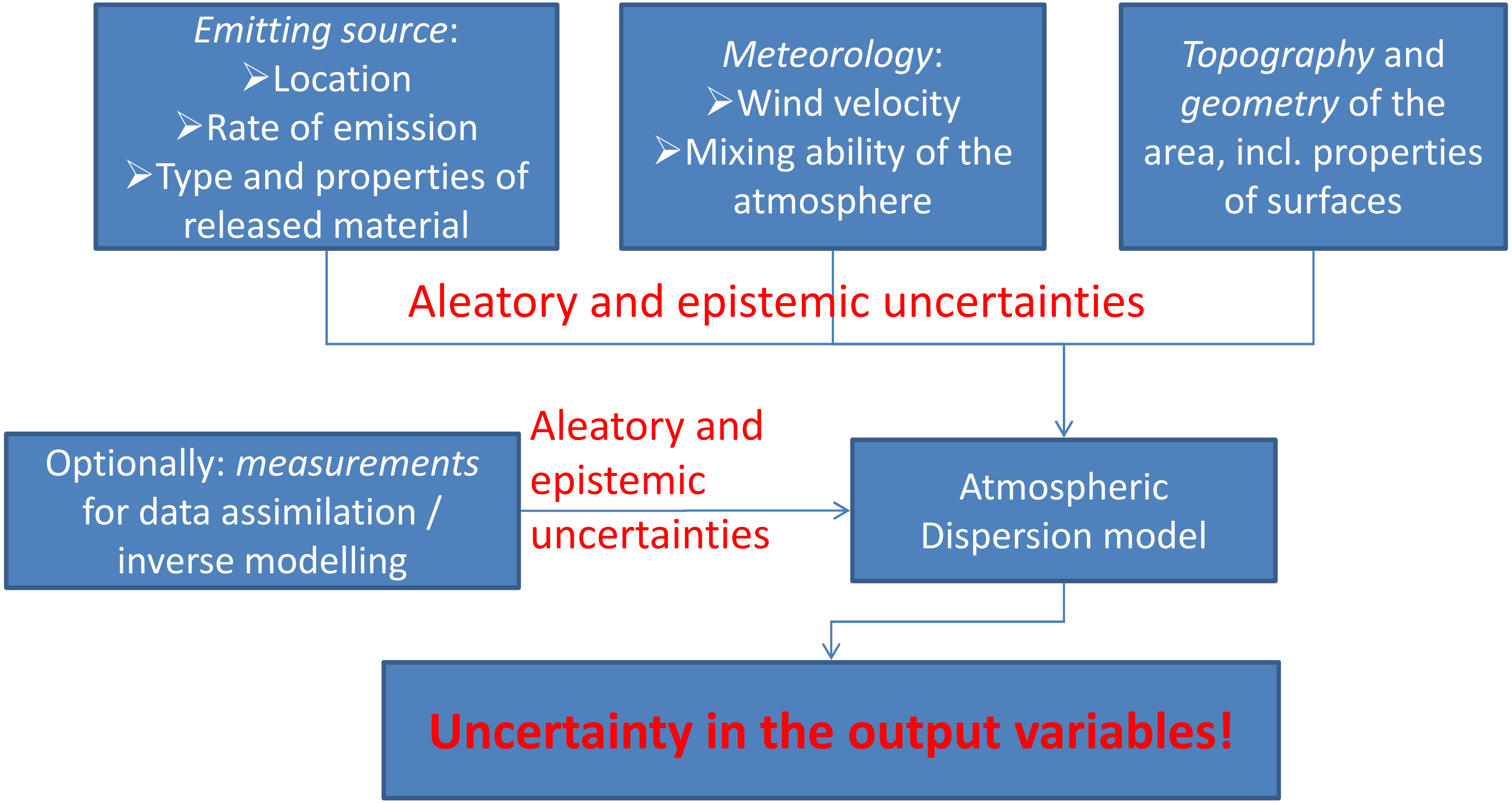
Aleatory uncertainty: uncertainty due to inherent randomness.

- inherent variation (variability) in a quantity
- can be treated in probabilistic framework (distributions)
- irreducible

Epistemic uncertainty: uncertainty due to lack of knowledge.

- can be eliminated in principle
- can not be treated in probabilistic framework (intervals)

Uncertainty quantification 3/3



Propagation of input uncertainties is an area of active research!

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Summary and Conclusions 1/2

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- There is already a wide range of wind flow and dispersion models of varying complexity, but research is still active
- Input and output requirements depend on the case and the model complexity
- Specific requirements are needed for short-range dispersion
- The appropriate selection depends on:
  - The characteristics of the specific case
  - The time phase in relation to a release of a hazardous substance
  - The available computational resources
- **Important scientific and practical issues remain for further research**
  - **Data assimilation / inverse modelling for emission estimation**
  - **Extreme values**
  - **Uncertainties**
  - **Speed of model execution**

Summary and Conclusions 2/2

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• **Quality assessment** of dispersion models used in emergency response systems at local scale requires **suitable**

✓ experimental data for validation,
✓ validation metrics,
✓ methods for the transfer of validation results to predictions.

• **Quality assurance protocol** of dispersion models used in emergency response systems at local scale should

✓ be general to be used for all 3 phases of emergency response,
✓ reflect the uncertainty in dispersion predictions,
✓ be widely accepted by creators and users of simulation results.

The present products

- **Database of measurements** available from experimental campaigns – *ongoing identification of useful ones for emergency response*

- **Inventory of emergency response tools and dispersion models** – *ongoing analysis on their appropriateness*

- **Package with validation metrics** – *ongoing selection of most appropriate for the evaluation of emergency response tools*

- **The COST ES1006 BACKGROUND AND JUSTIFICATION DOCUMENT**

Soon available on www.elizas.eu

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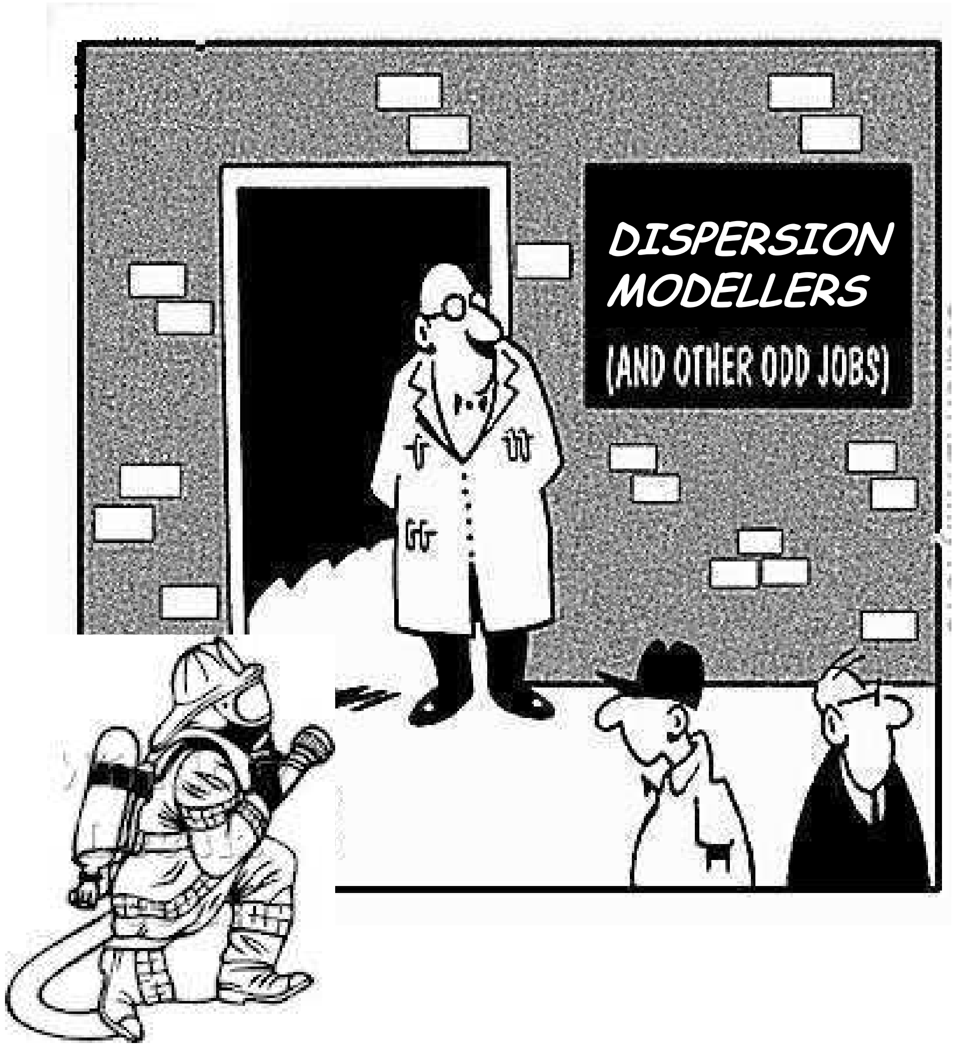
And now... Action!



A variety of emergency response tools is applied or is under development in different European Countries.

Research activities focusing on local-scale hazard dispersion are typically embedded in national research programs and generally lack a concerted approach at European level.

The **ES1006 COST Action** is intended to involve, support and harmonize the various existing national activities, extending the scientific focus towards short-term and local-scale threats, which most often concern the local emergency services.

An original purpose is to bring together scientists and emergency planning&response specialists, in order to evaluate and further develop the state-of-the-art scientific methodologies and to implement them in emergency response systems.

The non-competitive nature of **the Action** provides an environment in which:

- The limitations and uncertainties associated with current approaches to modelling for local-scale emergency response may be articulated;
- The most effective directions for future developments may be identified;
- A common strategy for improving the performance of modelling tools may be developed;
- High quality test data obtained in national research projects may be made available for validating and quantifying the uncertainties in models;
- The benefits from the research expertise available may be maximised and recommendations made from a broader scientific basis than national efforts alone could provide.

Overview of the modelling & operational challenges

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At the outset, mathematical models attempt to capture the physics of dispersion with various degrees of complexity

Once a set of equations has been derived, it must be solved using a numerical algorithm which determines the space / time precision of the solution

Reliability of dispersion computations also highly depends on the quality of input data:

- Description of the source term
- Meteorology at the scale of the event

The output of the dispersion modelling has to be translated into practical results used for CBRN impact assessments for the population and the rescue teams

Modelling must also be tractable within time constraints to assist in handling a crisis
The ultimate challenge is to meet the needs of first responders and decision makers

Among all these challenges, the importance of the quality and reliability of the dispersion modelling outputs for impact assessment can already be identified.

Concepts of FLOW and DISPERSION models

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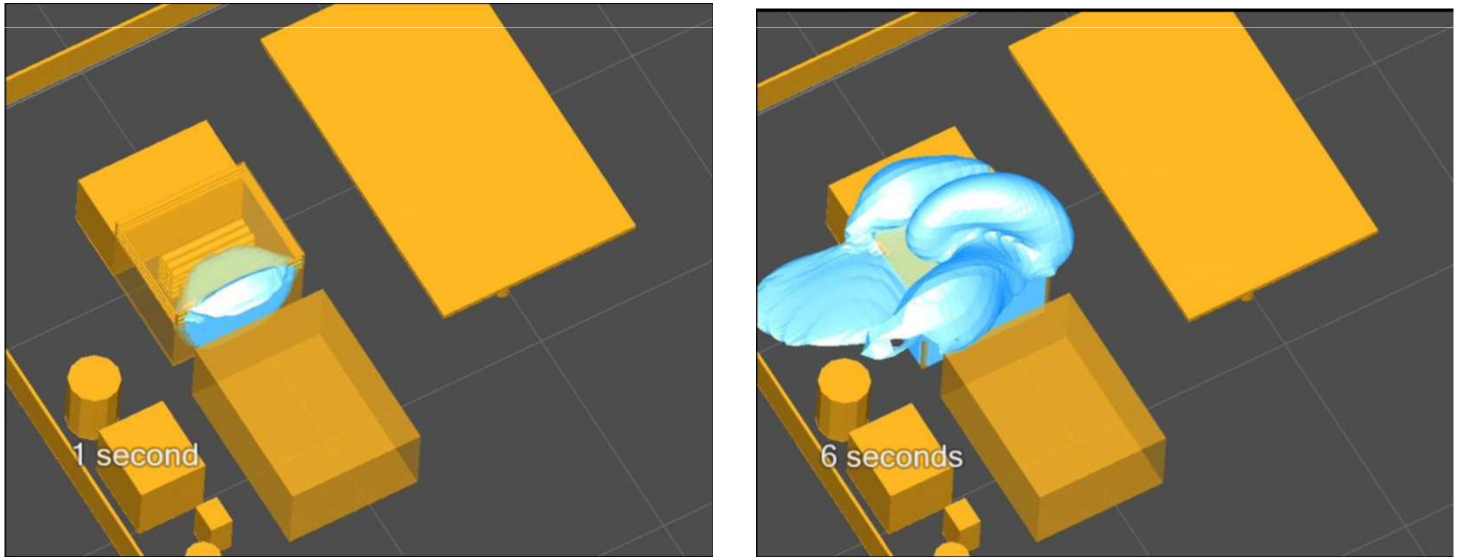
Important: is there any interaction between the existing atmospheric flow and the released hazardous substance?

No, the released substance does not influence the existing atmospheric flow

- ✓Passive tracer
- ✓Majority of real-world cases
- ✓Computations of flow and dispersion can be de-coupled

Yes, the released substance influences the existing atmospheric flow

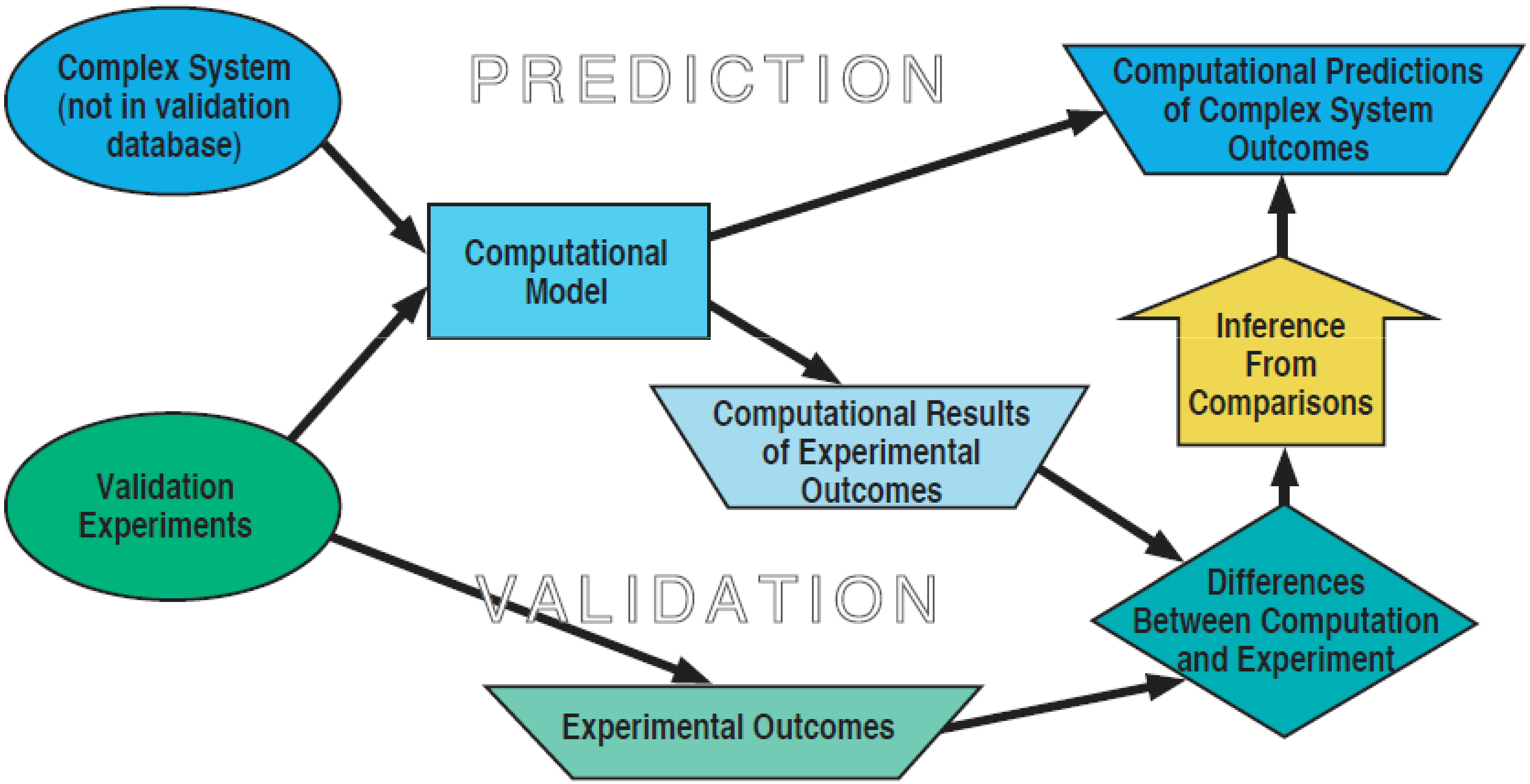
- ✓Interactions due to different density or temperature – buoyancy effects
- ✓Computations of flow and dispersion should be performed simultaneously



Example of computation of hydrogen release from a re-fueling station: buoyant gas affecting the flow field

Quality assurance in computational modelling

Prediction



(Oberkampf et al., 2002)