MODERN COMPUTATIONAL ORACLES

IN

CHEMICAL ENGINEERING

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Symposium on New Frontiers in Chemical and Biochemical Engineering
Thessaloniki, 26-27 November 2009

Outline of the argument

- *"What will happen if…?"*
  is the most important question which a conscious being can ask.

  Answering it rightly more times than not is what keeps most of us safe, healthy and reasonably prosperous; for it allows us to:

  ▪ **foresee**, and so avoid, dangerous events;

  ▪ **select**, from available options, those which best promote happiness and well-being;

  and

  ▪ create opportunities which **never before existed**

Outline of the argument

- Society seeks, through education,
  - to inculcate in the young **the habit of asking** this question;

    and
  - to convey **how** the right answers can be arrived at, which means to teach to all: **techniques of prediction**.
- In essence, all such techniques are the same: examine the past; and if elements of the present are seen there, suppose that what transpired is likely to happen again.
- Thus: “When last I pulled the tail of a cat, it scratched me; so, if I do it again, another scratch is what I must expect”.
  It is a sound principle.

Outline of the argument

- In ancient times, **oracles** were consulted on matters of importance, as best fitted by age, experience or connections **to foresee, what the past implied about the impending future**.
- That too was a sound principle, for those who could afford the oracle’s fees!
- How are these principles applied in Chemical Engineering?
  - If the task in hand involves little novelty, as when one more reactor is to be built for an established and satisfactory production line, simple repetition of past actions is what the principle dictates.
  - But when the performance requirements have changed, exceeding what the old reactor is capable of, **novelty** is needed; and **what is new has**, by definition, **no past to be examined**.
- What to do?

Outline of the argument

- There is however a more **general encapsulation of the past**, which we call **science**; and for chemical engineers it takes the form of:

  - laws of **conservation of mass, momentum and energy**, (Lomonosov, Newton, Joule);
  - laws of **transport** of those same entities by diffusion, viscous action and heat conduction (Fick, Newton, Fourier);
  - laws of deformation of solids in response to mechanical and thermal stresses (Hooke);
  - laws governing **rates** of **chemical** transformation, and **electrical** and **magnetic** interactions (Arrhenius, Faraday).

- It is such laws, to which the chemical engineer must turn, whenever actions without precedent are contemplated, in order to answer “what will happen if…?” questions.

Contents of the lecture

The present lecture explains:

- how **simulation-by-computer** has become the engineers’ favored **prediction technique**,
  and
- how specialized **software packages** have become the **oracles** which they consult.

- Two things the modern oracles share with the ancient ones:

  - they **cost** money (or sheep, oxen or other currency);
  and
  - Their pronouncements are **never 100% reliable**.

- The reasons for both will be explained.

CONSERVATION EQUATIONS FOR ONE- AND TWO-PHASE FLOWS

- Notation :
  - r = volume fraction;
  - div = divergence operator;
  - ϱ = density;
  - m = mass source per unit volume;
  - V = velocity vector; i = phase
- Conservation of phase mass

$$\frac{\partial}{\partial t}(\rho_i r_i) + div(\rho_i r_i \vec{V}_i) = \dot{m}_i$$

- "Overall" mass-conservation equation
  - ☆ Summation over all phases leads to :

$$\sum_{i=1}^{n}\left(\frac{\partial}{\partial t}(\rho_i r_i) + div(\rho_i r_i \vec{V}_i)\right) = 0$$

- For two-phase flow $r_1 + r_2 = 1$
- Phases distinguished not only in thermodynamic terms eg. upward/downward/sideways moving fluid; small/medium/large particle sizes.

THE GENERAL Φ-EQUATION

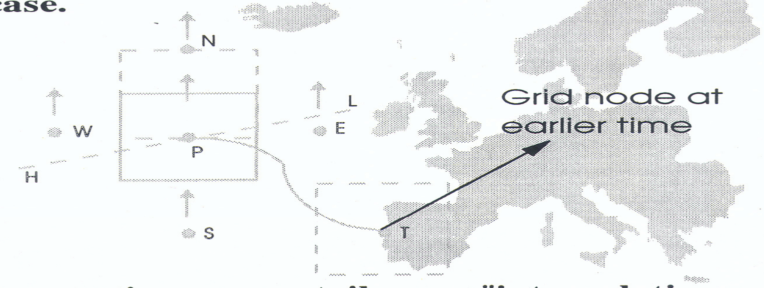
- Notation:
  - Φ = The general conserved property;
  - S_Φ = Source of Φ per unit phase volume;
  - Γ_Φ = exchange coefficient;
  - Φ = Φ-content of material crossing phase boundary.
- The general source-balance equation for Φ is:

$$\frac{\partial}{\partial t}(\rho_i r_i \Phi_i) + div(\rho_i r_i \vec{V}_i \Phi_i - r_i \Gamma_\Phi grad\Phi) = \dot{m}_i \Phi_i + r_i S_{\Phi_i}$$

- Equations for the various quantities differ primarily in the way in which the terms Φ and S are connected with other variables.
- Distribution of effects between $m_i \Phi_i$ and S_i is sometimes arbitrary.
- Impartiality between phases and velocities is a desideratum. All variables are essentially statistical and much can be said about different methods of forming the averages they represent.

FINITE-DOMAIN EQUATIONS, 1. FORMULATION

- Finite-domain equations are derived by integration of the differential equations over finite control volumes ("cells" or "sub-domains").
- The cells are "topologically Cartesian", having six sides and eight corners in the 3D case.



- Integration entails "interpolation assumptions" about Φ values, and values of Φ gradients, prevailing at cell boundaries.
- Cells and nodes for velocity components are "staggered" relative to those for all other variables.

FINITE-DOMAIN EQUATIONS, 2. FORMULATION

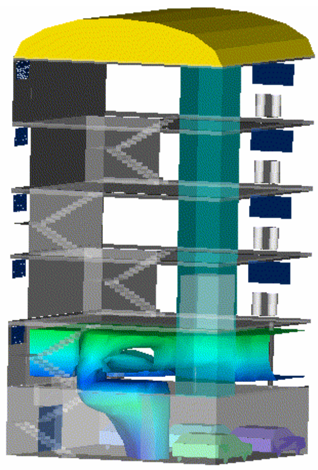
- Differ from Finite-Differences :
  - origin (no Taylor series expansion used)
  - values of coefficients as a consequence
- Differ from Finite-Elements :
  - origin (neither variational principle nor Galerkin weighting used)
  - number of nodes referred to (6 for 3D); usually more in Finite-Element methods)

Fire Simulation

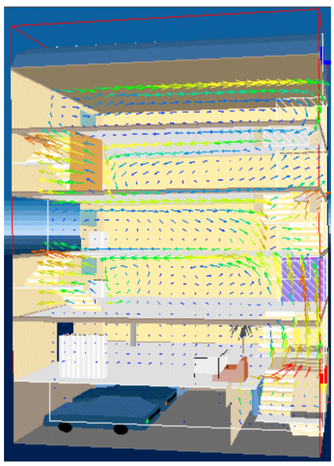
- industry
- buildings
- public transport
- forests

! need for designing reliable systems for fire extinction

Fire simulation in a building

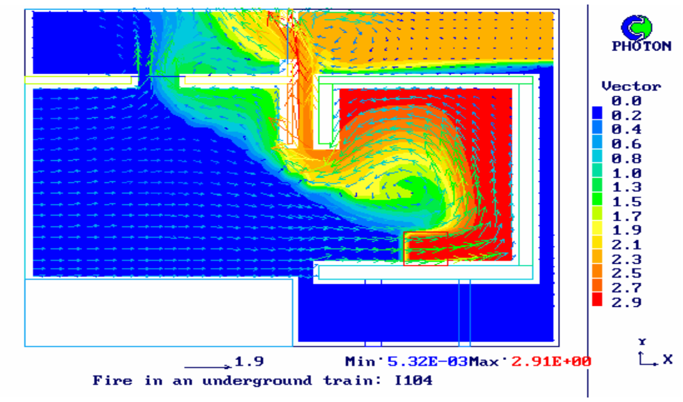


isosurface of temperature



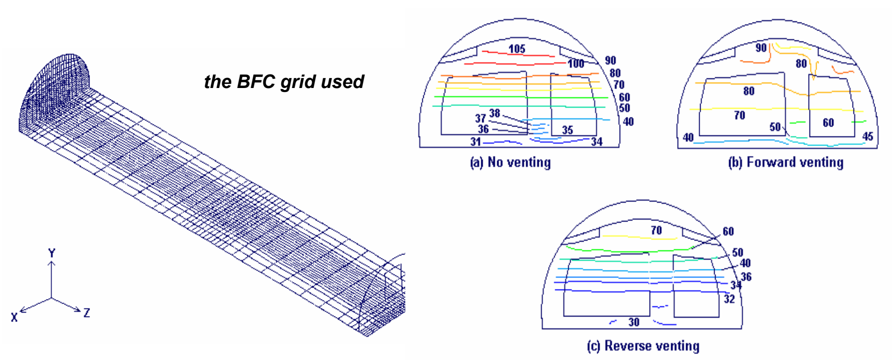
velocity vectors in a vertical cross-section

Fire simulation at a METRO station

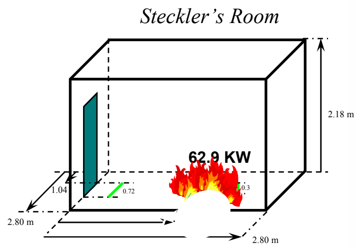


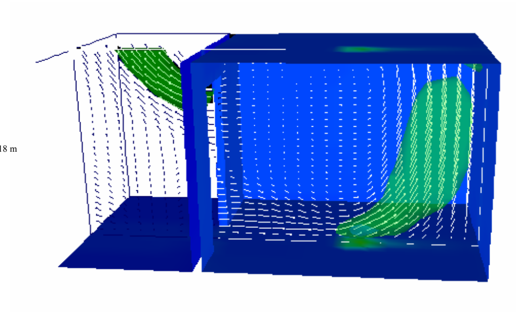
Fire simulation in an airplane cabin

temperature contours

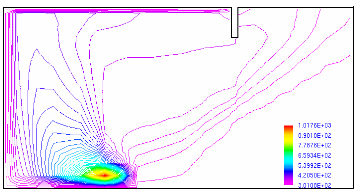


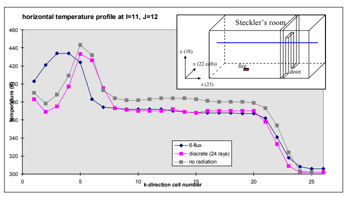
Fire simulation in a room

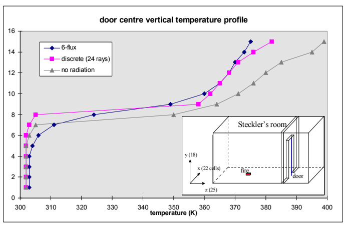


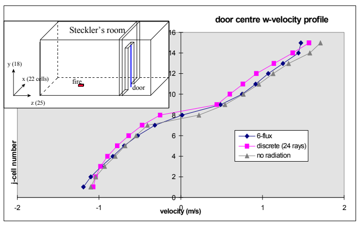


Fire simulation - Results



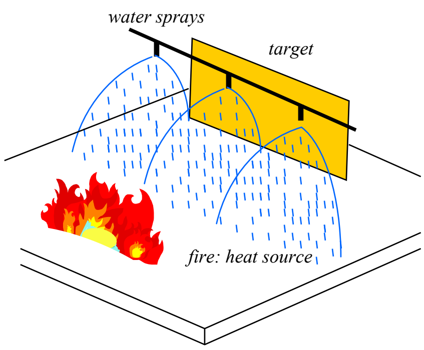


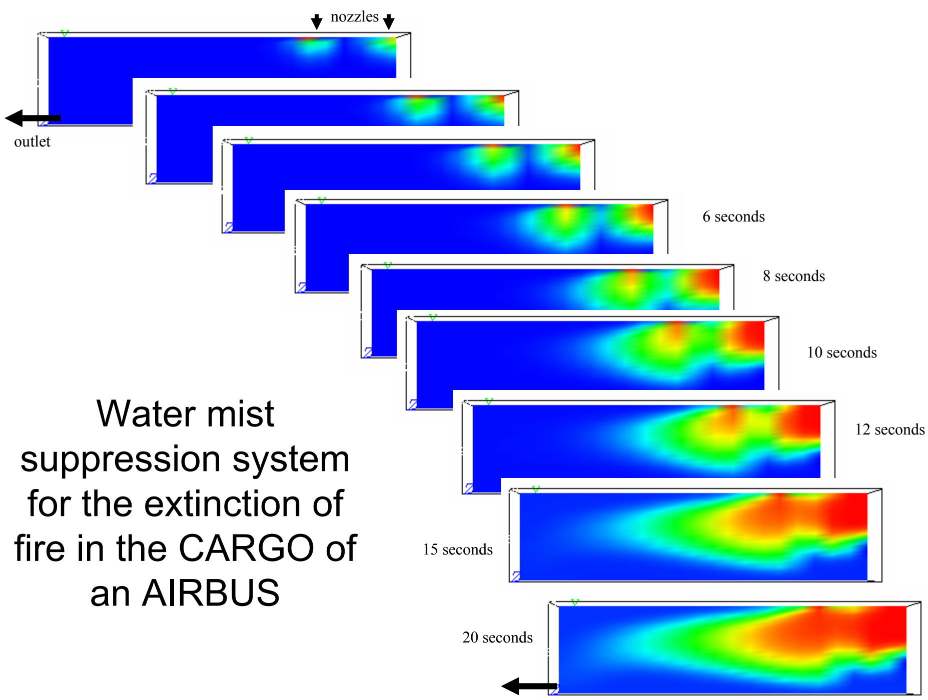




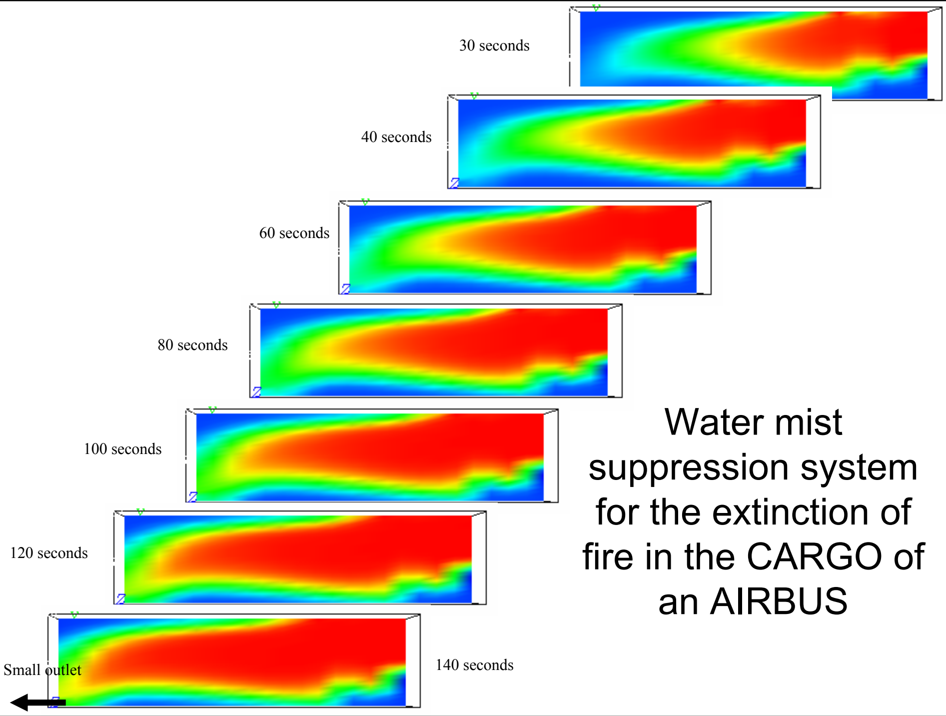
Water mist suppression system

- Fine water spray systems have received much attention as a fire suppression system
- Radiation is attenuated due to absorption by the water droplets
- Water sprays can even be used as radiative shields for protecting from possible secondary ignition due to thermal radiation



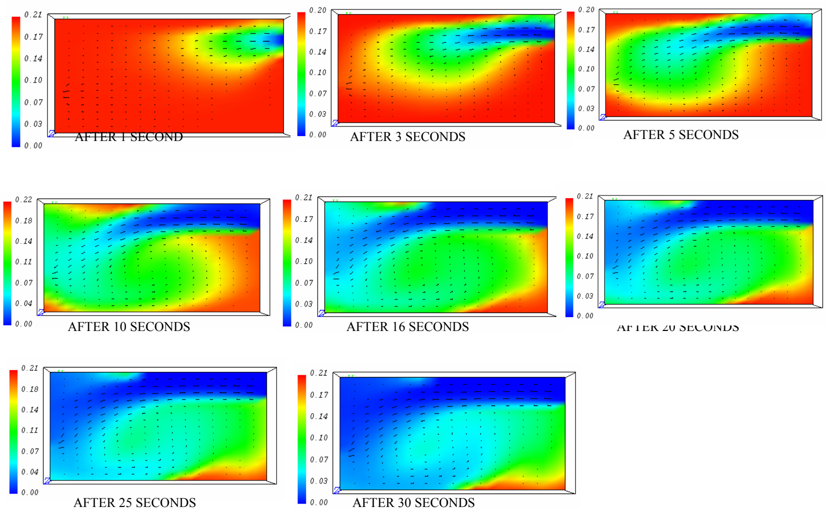


Water mist suppression system for the extinction of fire in the CARGO of an AIRBUS



Water mist suppression system for the extinction of fire in the CARGO of an AIRBUS

Simulation of ejection of Inert Gas (NEA-AirLiquide) for the extinction of fire at the CARGO of an AIRBUS

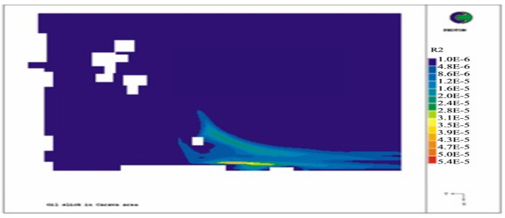


Simulation of an Oil-Spill

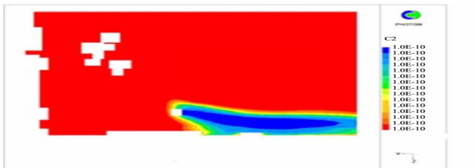
Prasologos island

(included in the NATURA 2000 network)

- The oil spill at the surface of the sea 3h after the accident



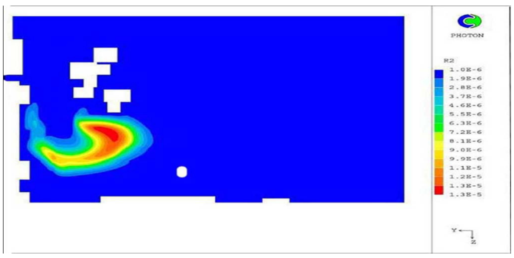
- The emulsion at the surface of the sea 3h after the accident



Simulation of an Oil-Spill

Lesvos island

- The oil spill at the surface of the sea 10s after the accident

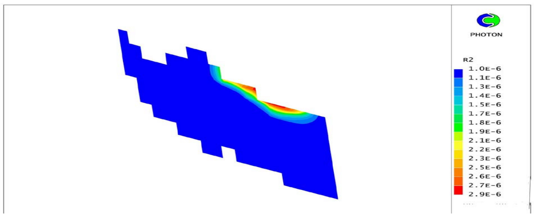


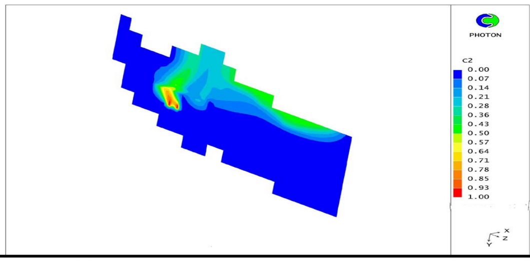
- The oil spill at the surface of the sea 6.5h after the accident

Simulation of an Oil-Spill

Euboean gulf

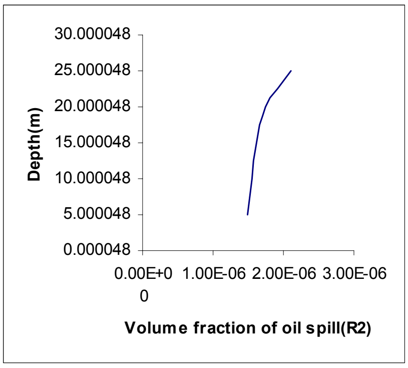
- The oil spill at the surface of the sea 12h after the accident

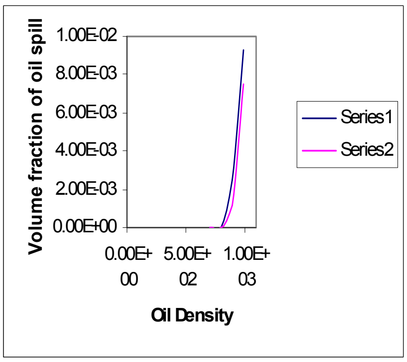




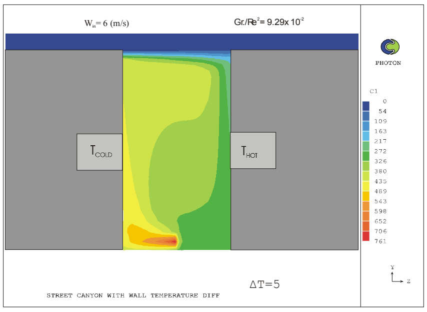
- The emulsion at the surface of the sea 12h after the accident

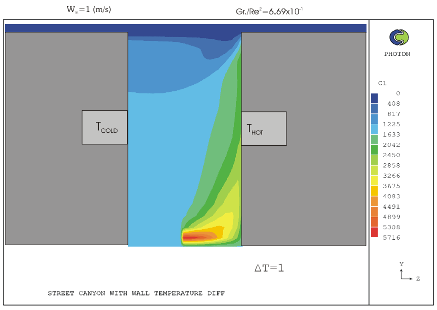
Simulation of an Oil-Spill



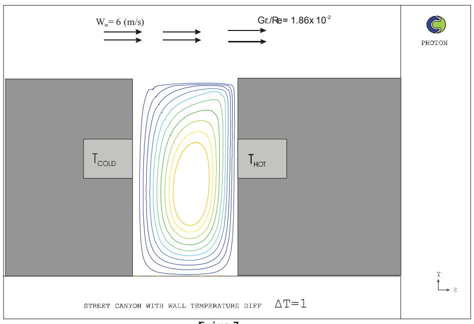


Air pollution - street canyon

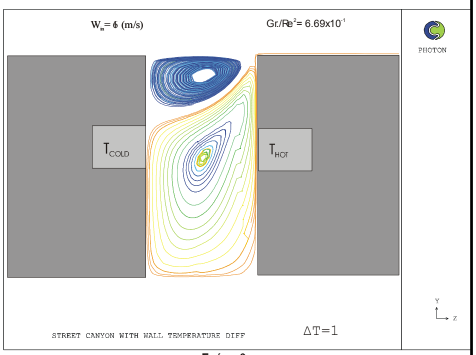




Air pollution - street canyon

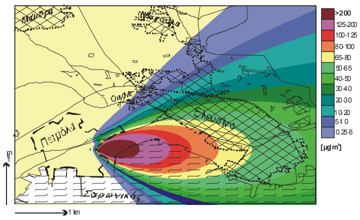


Σχήμα 7

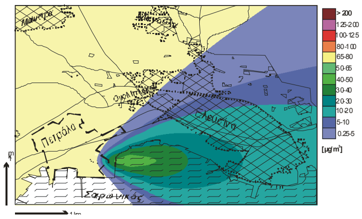


Σχήμα 9

Environmental impact of an Oil Refinery

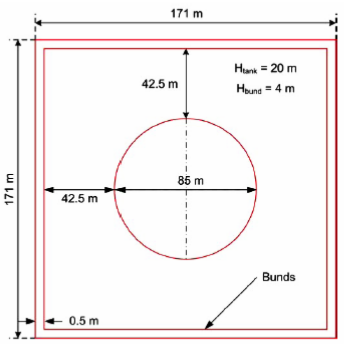


SO_2 daily concentration zones.
Existing situation.
(westerly wind at 2 m/s, equilibrium class A, Inersion height 400 m).

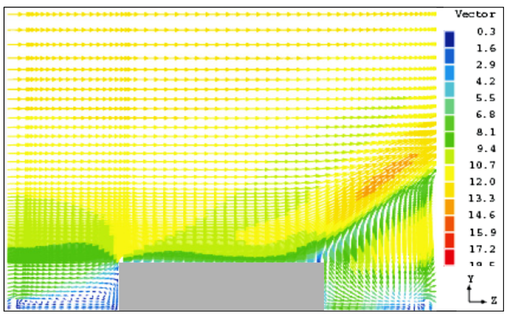


SO_2 daily concentration zones.
Future situation.
(westerly wind at 2 m/s, equilibrium class A, Inersion height 400 m).

Fuel-tank Fires

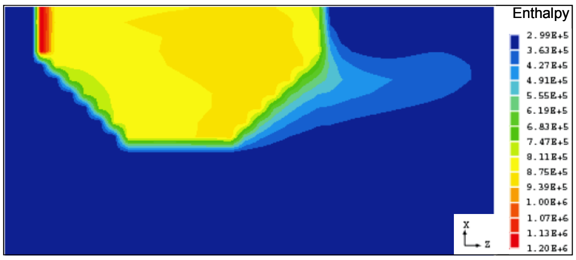


The tank geometry considered.

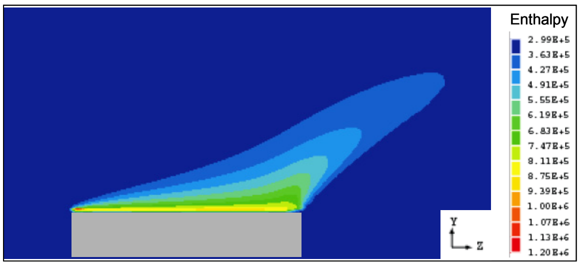


Velocity Vectors (YZ plane)

Fuel-tank Fires

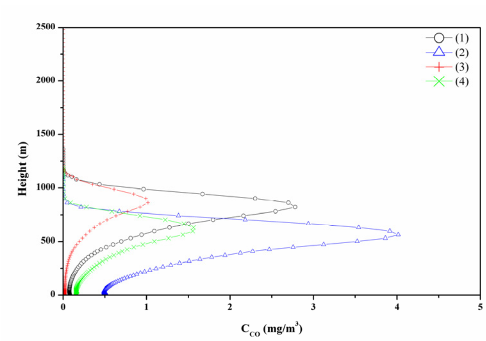


Enthalpy Contours (XZ plane)

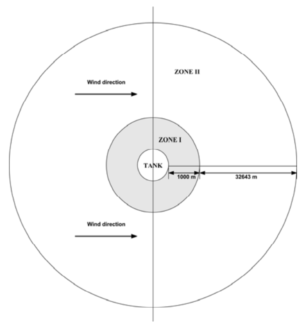


Enthalpy Contours (YZ plane)

Fuel-tank Fires

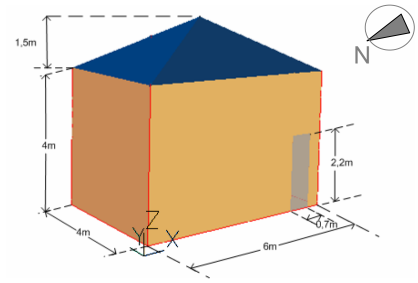


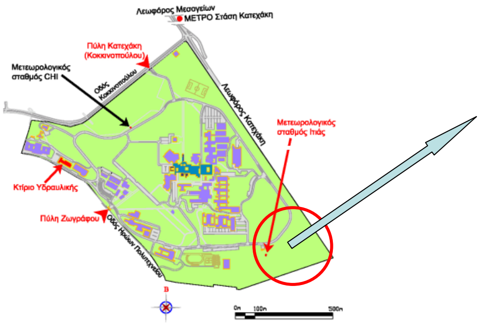
Concentration of CO vs. the height at a position of 5 km from the flow axis.



Configuration of risk zones I and II.

Πρότυπο Κτίριο-Ιδεατός Τόπος



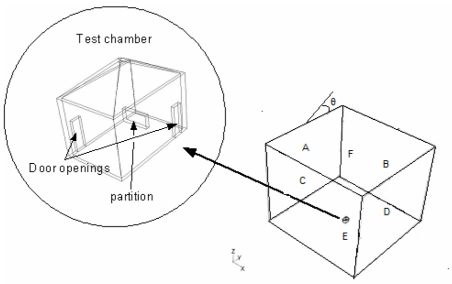


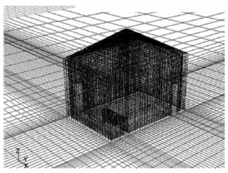
- ✓ Αραιοκατοικημένη Περιοχή
- ✓ Περιοχή Απαλλαγμένη από Θερμικές Πηγές
- ✓ Ημιαστικό Περιβάλλον

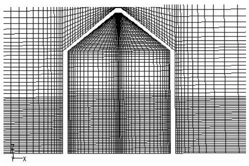
Κτίριο Εξοχικού Τύπου

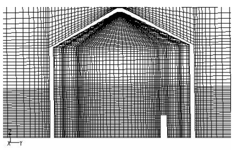
(rural-type building)

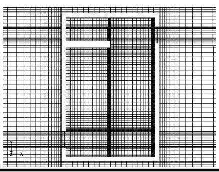
Computational domain and grid



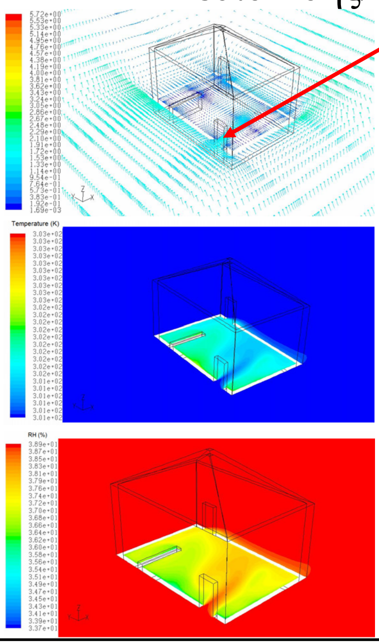








Πεδίο Ροής/Βιοκλιματικοί Χάρτες



Επιτάχυνση ροής

PMVs ↓, PD ↑ στο άνοιγμα

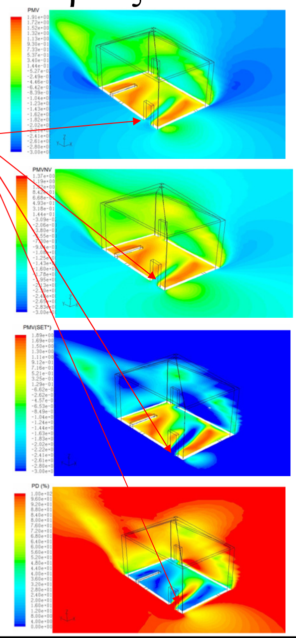
Αποδεκτές συνθήκες

-0.88<PMV<0.88

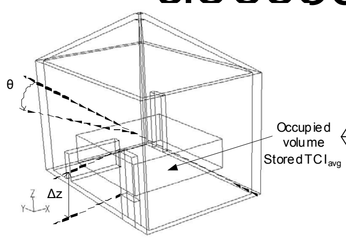
AND

PD<15%

Venturi Effect!!!



Βάση Δεδομένων-Μεταβλητές εισόδου/εξόδου



M=70W/m², Height O.V.=1.1-1.8m

M=60W/m², Height O.V.=0.6-1.2m

M=40W/m², Height O.V.=0.4-0.7m

✓ Βήμα Προσανατολισμού: Δθ=30°

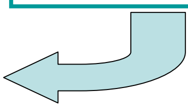
✓ Βήμα Ύψους Ανοίγματος: Δz=0.275m

63 (+ 10) ζεύγη Μεταβλητών Εισόδου/Εξόδου για κάθε δραστηριότητα!

Διάνυσμα εισόδου: $\vec{x} = [\theta \ \ \Delta z]^T$

Διάνυσμα εξόδου: $\vec{y} = [PMV \ \ PMV_{NV} \ \ PMV(SET^*) \ \ PD]^T$

No. of data	*PMV*	*PMVNV*	*PMV(SET*)*	*PD* (%)	*θ* (degrees)	*Δz* (m)
1	1.4785	1.0159	1.5506	5.7482	0	2.2
2	1.4278	0.9618	1.3633	7.2892	30	2.2
3	1.2340	0.8107	1.0907	14.7745	60	1.925
4	1.3651	0.9146	1.2710	12.9148	90	1.375
-	-	-	-	-	-	-
-	1.2325	0.8270	0.9893	22.0853	120	1.1
-	-	-	-	-	-	-
-	1.2629	0.8579	0.9426	21.6496	150	0.825
-	-	-	-	-	-	-
63	1.5157	1.0460	1.6218	4.2040	180	0



Βάση Δεδομένων-Μεταβλητές εισόδου/εξόδου

Εκπαίδευση/Επαλήθευση Τεχνητού Νευρωνικού Δικτύου

$\vec{y} = f(\vec{x})$

M=70W/m², Height O.V.=1.1-1.8m

Σύνολο Ελέγχου Ακρίβειας Τ.Ν.Δ. .2m

Kennard-Stone

M=40W/m², Height O.V.=0.4-0.7m

✓ Βήμα Προσανατολισμού: Δθ=30°

✓ Βήμα Ύψους Ανοίγματος: Δz=0.275m

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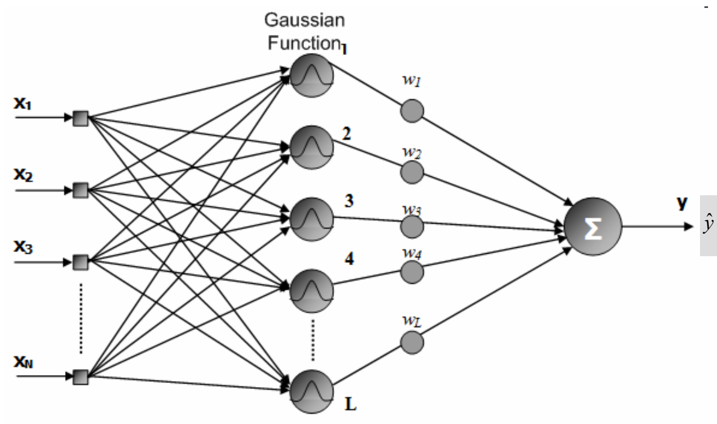
-	1.2325	0.8270	0.9893	22.0853	120	1.1
-	-	-	-	-	-	-
-	1.2629	0.8579	0.9426	21.6496	150	0.825
-	-	-	-	-	-	-
63	1.5157	1.0460	1.6218	4.2040	180	0

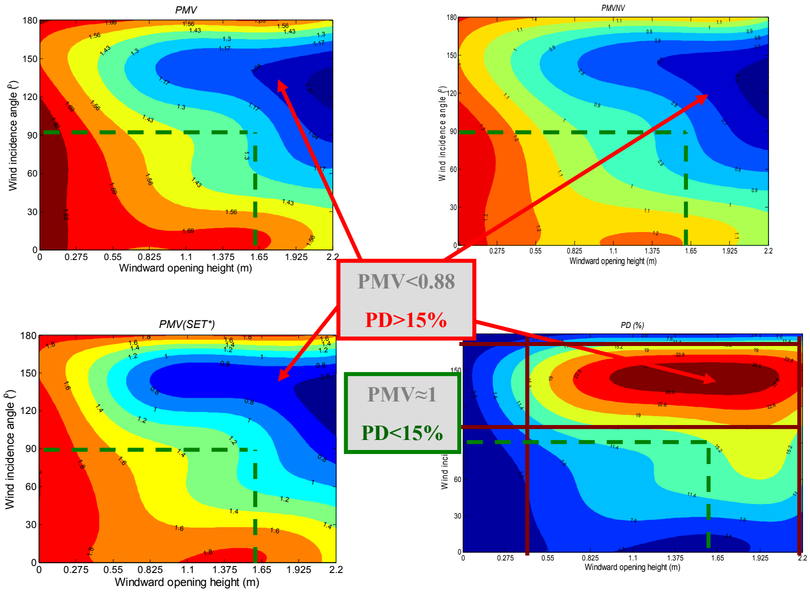
Δομή Τεχνητού Νευρωνικού Δικτύου



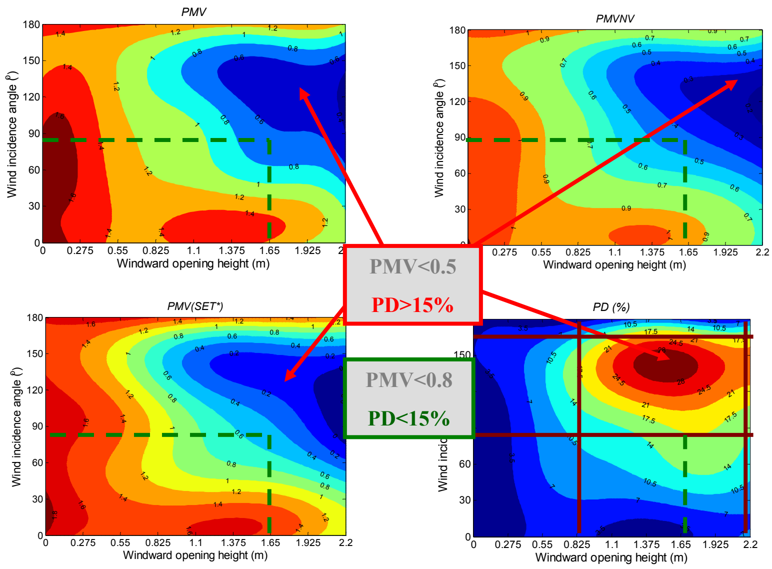
$$\hat{y}(\mathbf{x}^i) = \sum_{j=1}^{L} w_j f\left(\left\|\mathbf{x}^i - \mathbf{c}^j\right\|\right)$$

$$f\left(\left\|x^i - c^j\right\|\right)$$

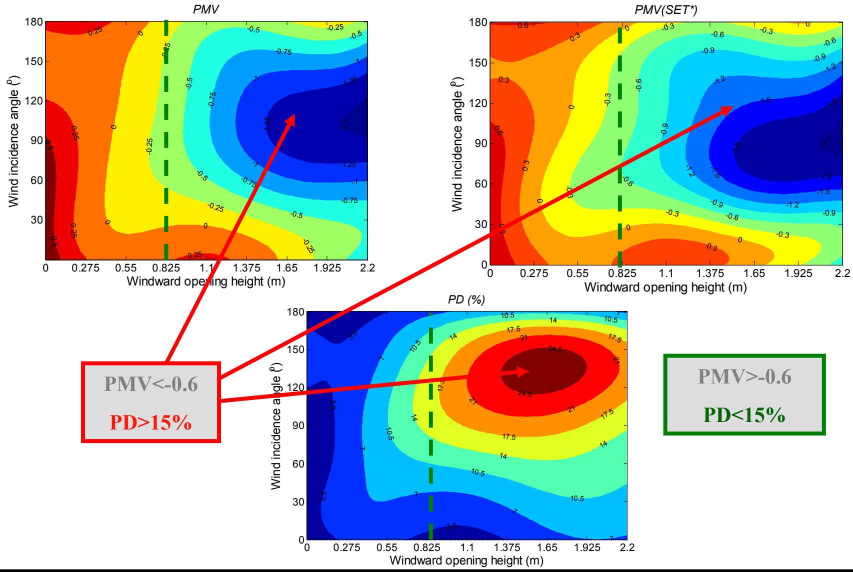
Αποτελέσματα/Πρόβλεψη
M=70W/m2



Αποτελέσματα/Πρόβλεψη
M=60W/m2



Αποτελέσματα/Πρόβλεψη
M=40W/m2



The cost of CFD

- The new **oracles** demand their sacrifices

  What are they?

  1. The software

  In the first two decades of the CFD industry, **licences** to use the software packages could be sold for tens of thousands of Euros.

  Nowadays their price is dozens times less.

  Industrial organizations can purchase them easily, **academic ones** not so as yet.

The cost of CFD

2. The hardware

- Nowadays hardware costs have decreased dramatically and **parallel-computing** facilitates the use of **more adequate computational** grids
- Another possibility is to use **remote clusters** via Internet paying for actual services.

In this case it is **only a laptop** that a user needs to solve great multifactor problems.

The Cost of CFD

3. The personnel

- Nowadays, therefore, it is the **cost** of hiring CFD-literate **personnel** which is the **most serious impediment** to the extension of computer simulation.
- **Suitable** people are those,

▪ who have experience of **several** packages

▪ who recognize that most of their claims to superiority are ill-founded,

▪ who **understand the limitations** from which they all suffer

▪ who possess **well-balanced commonsense**, and

▪ who are **pragmatically skeptical** and when the occasion arises, they can conclude that

"A particular computer simulation simply must be wrong"

Why the "Oracles" are not completely reliable

- Grids are inadequate. If a hundred **million** control cells had been used, these cells would still be hardly small enough to represent a **continuous problem** as discrete. Only the largest computer clusters in the world would have been able to handle so many; and the computation would take **for too long** for its outcome to remain of interest.
- **Engineers** like to think that fuel and oxygen combining form "combustion product" gases but **chemists** have discovered that a great many of **intermediate products** are formed in combustion, and the information is **too immense**.
- Therefore, engineers create **simplified combustion models** and their accuracy always raises doubts.
- The same is true for many physical phenomena such as radiation and turbulence

Why the "Oracles" are not completely reliable

- Although turbulence has been much studied, none of the current representations **are known to correspond with reality** in all circumstances.
- This regrettable fact seems likely to remain until some Newton reduces chaos to order.
- Until then all predictions of turbulent flows must be regarded as no more than probable forecasts of "What will happen if…?"
- When **chemical reaction** and two-phase effects are present the **margin for error widens.**

Why the "Oracles" are not completely reliable
What is to be done?

- **The optimists** are impressed by the **plausible-seeming attractively-coloured** images they produce.
- The pessimists argue that all packages use the **same dubious models** of turbulence, etc, and all are compelled to use **far-too-coarse grids.**

Aristotle's advice is here appropriate: The best lies between the **extremes**
It entails recognizing that

1. the CFD-based predictions are no more than **indicators** of probability, but
2. they are **immensely better** than the mere guess-work which is mankind's only alternative

Conclusions

- The use of CFD has been **increasing steadily** in the last three decades for the design of equipment and processes of modern engineering
- Its use seems certain to **continue to grow**
- It is therefore obvious that the educational systems of the **world** should prepare their students to **participate** and to **contribute** to it.

CONCLUSIONS

- ▶ Methods now exist for computing complex phenomena with a view of protecting the Environment, saving energy and controlling major hazards.
- ▶ Detailed improvement of modeling, and computer processing is continuous, as more reliable physical information becomes available.
- ▶ Two-phase computational methods are now as advanced as single-phase ones. It is now feasible to compute for two or more "interpenetrating continua" in 1-, 2-, or 3-dimensions.
- ▶ Predictions to-date are encouraging. Further validation of codes is needed; this requires reliable data for complex flows.
- ▶ Uncertainty remains for turbulent transport and combustion in single and particularly in two-phase flows. Hypotheses are needed, guided by experimental observations. Numerical computations can effect the comparisons.