CFD in Environmental Engineering and risk analysis.

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Abstract: This paper describes the mathematical modeling and associated computer simulations of environmental problems related to flow and heat/mass transfer. Many key "issues" in designing environmental protection systems, and in performing environmental risk assessment and control, are related to the behavior of fluids in turbulent flow, often involving more than one phase, with chemical reaction or heat transfer. Computational-Fluid-Dynamics (CFD) techniques have shown great potential for analyzing these processes and are very valuable to the environmental engineer and scientist, by reducing the need to resort to "cut and try" approaches to the design of complex environmental-protection systems and to any relevant decision-making process. Multi-dimensional, multiphase dynamic models for the dispersion of air, water and soil pollutants and for the prediction of environmental risks are presented. Results using model simulations are presented for some cases of atmospheric and marine pollution, as well as for the environmental risks of fires and of petrol-tank explosions. It is concluded that the results are physically plausible and can be used with confidence. Air, water and soil management systems can be improved by the application of these computational prediction techniques.

Keywords: Environmental; dynamic modeling; turbulence; pollutants dispersion; CFD; fires; explosions; risk assessment; atmospheric pollution; marine pollution.

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1. Introduction

Computers and computational methods have been used since the early 1970's to approach engineering problems in design, control and operations [1-3]. Progress has been slower in the environmental field of applications, as the scale of the environmental problems is orders of magnitude larger than that of equipment design, therefore, awaited the appearance of large-capacity computers and/or sophisticated solvers and techniques, as for example parallel processing [4-5].

The modern computer's ability to handle complex mathematics and to permit the solution of detailed models allows present-day scientists, engineers and policy makers to model environmental process physics and chemistry at all scales, to construct models that incorporate all relevant phenomena (emissions, diffusion, convection, radiation, chemical reaction, etc.) and optimize, more on the basis of computed theoretical predictions and less on empirical. This development allows us to-day to conduct, for example, the prediction of Volatile Organic Compounds (VOC) dispersion emitted from flooring materials in buildings [6]; the prediction and control of water pollution in Trans Boundary Ecosystems, and environmental risk assessment and emission control [7].

Apart from air and water quality studies, the models must be also capable of being used in other environmental applications as well, e.g. in porous media or, in general, in the subsurface [8].

In summary, the mathematical model we present can simulate environmental problems ranging from simple pollutant-diffusion assessments to complex multi-dimensional, multiphase applications, for the purposes of:

- Prediction/evaluation of environmental dispersions/spills
- Evaluation of environmental changes
- Evaluation of thermal discharges

- Temperature modeling
- Evaluation of atmospheric pollutants transport
- Evaluation of water and soil contaminant transport
- Determination of maximum ground-level concentrations
- Computation of effective stack height
- Prediction of particulate distributions outdoors and indoors
- Prediction of deposition of particulate matter from stacks, etc.
- Estimation of industrial emissions impact
- Modeling of emissions from landfills
- Modeling of atmospheric impacts from mobile sources.
- Computation of the release of VOCs from petroleum storage tanks and from wastewater treatment plants
- Modeling contaminants fate in aquatic ecosystems
- Modeling CO_2 sequestration in geological formation
- Performing risk assessments in cases, for example, of fires in buildings/forests/public transport, etc., pool fires or/and explosions in industrial storage tanks, etc.

It is obvious from the above arguments that the process of modeling as described above can (and must) serve also a consensus-building function. It can help to build mutual understanding, solicit and test input from a broad range of stakeholder groups, and sustain dialog between members of these groups, by presenting objective scientific findings rather than individual beliefs that may be biased, and cause disagreements.

2. The Mathematical Modelling

2.1 The Differential Equations

A convenient assumption, based on the concepts of time- and space-averaging, is that more than one phase can exist at the same location at the same time. Then, any small volume of the domain of interest can be imagined as containing, at any particular time, a volume fraction r_i of the i-th phase. As a consequence, if there are n phases in total,

$$\sum_{i=1}^{n} r_i = 1 \qquad (1)$$

When flow properties are to be computed over finite time intervals, a suitable averaging over space and time must be carried out.

Following the above notion, that treats each phase as a continuum in the domain of interest, we can derive the following balance equations:

- **Conservation of phase mass**

$$\frac{\partial}{\partial t}(\rho_i\, r_i) + \mathrm{div}\left(\rho_i\, r_i\, \vec{V_i}\right) = \dot{m}_i \qquad (2)$$

Where ρ_i is the density, $\vec{V_i}$ is the velocity vector, r_i is the volume fraction of phase; $\dot{m}_i$ is the mass per unit volume entering the phase, from all sources per unit time, and *div* is the divergence operator (i.e. the limit of the outflow divided by the volume as the volume tends to zero).

Summation of (2) over all phases leads to the "over-all" mass-conservation equation:

$$\sum_{i=1}^{n}\left[\frac{\partial}{\partial t}(\rho_i\, r_i) + \mathrm{div}\left(\rho_i\, r_i\, \vec{V_i}\right)\right] = 0 \qquad (3)$$

which has of course a zero on the right-hand side.

- **Conservation of phase momentum**

$$\frac{\partial}{\partial t}(\rho_i\, r_i u_{ik}) + \mathrm{div}\left(\rho_i\, r_i\, \vec{V_i} u_{ik}\right) = r_i\left(-\vec{k}\cdot \mathrm{grad}\, p + B_{ik}\right) + F_{ik} + l_{ik} \qquad (4)$$

Where: u_{ik} is the velocity component in the direction k of phase i; p is pressure, assumed to be shared between the phases; $\vec{k}$ is a unit vector in the k-direction; B_{ik} is the k-direction body force per unit volume of phase I; F_{ik} is the friction force exerted on phase i by viscous action within that phase; and l_{ik} is the momentum transfer to phase i from interactions with other phases occupying the same space.

- **Conservation of phase energy**

$$\frac{\partial}{\partial t}(r_i(\rho_i\, h_i - p)) + \mathrm{div}\left(\rho_i\, r_i\, \vec{V_i} h_i\right) = r_i Q_i + H_i + J_i \qquad (5)$$

Where: h_i is stagnation enthalpy of phase i per unit mass (i.e. the thermodynamic enthalpy plus the kinetic energy of the phase plus any

potential energy); Q_i is the heat transfer to phase i per unit volume; H_i is heat transfer within the same phase, e.g. by thermal conduction and viscous action; and J_i is the effect of interactions with other phases.

- **Conservation of species-in-phase mass**

$$\frac{\partial}{\partial t}(\rho_i r_i m_{il}) + \mathrm{div}\left(\rho_i r_i \vec{V}_i m_{il}\right) = \mathrm{div}(r_i \Gamma_{il} \mathrm{grad}\, m_{il}) + r_i R_{il} + \dot{m}_i M_{il} \quad (6)$$

Where: m_{il} is the mass fraction of chemical species l present in phase i; R_{il} is the rate of production of species l, by chemical reaction, per unit volume of phase i present; Γ_{il} is the exchange coefficient of species l (diffusion); and M_{il} is the l-fraction of the mass crossing the phase boundary, i.e. it represents the effect of interactions with other phases.

All of the above equations can be expressed in a single form as follows:

$$\frac{\partial}{\partial t}(\rho_i r_i \varphi_i) + \mathrm{div}\left(\rho_i r_i \vec{V}_i \varphi_i\right) = \mathrm{div}\left(r_i \Gamma_{\varphi i} \mathrm{grad}\, \varphi_i\right) + \dot{m}_i \Phi_i + r_i s_{\varphi i} \equiv \text{total source of } \varphi_i \quad (7)$$

Where: φ_i is any extensive fluid property; the first term on the right-hand side expresses the whole of that part of the source term which can be so expressed, with $\Gamma_{\varphi i}$ being the exchange coefficient for φ_i. $s_{\varphi i}$ is the source/sink term for φ_i, per unit phase volume; and $\dot{m}_i \Phi_i$ represents the contribution to the total source of any interactions between the phases, such as nay phase change (with Φ_i being the value of φ_i in the material crossing the phase boundary, during phase change). Distribution of effects between $\dot{m}_i \Phi_i$ and $s_{\varphi i}$ is sometimes arbitrary, reflecting modelling convenience. For single-phase situations, the above equations are valid by setting the *r's* to unity.

For turbulent flow, averaging over times which are large compared with the fluctuation time leads to similar equations for time-average values of φ_i with fluctuating-velocity effects usually represented by enlargement of $\Gamma_{\varphi i}$. More details on the above concepts and equations may be found in [9-13].

There is much experience to prove that the mathematical model, as formulated above, does have unique solutions, to which the solutions of the relevant finite-domain equations do converge as the time step and grid spacing become small. The present paper provides further confirmation of this aspect of the model.

2.2 Auxiliary relations and boundary conditions

The above set of differential equations is solved normally together with auxiliary relations that express physical laws of various kinds. For example, equations of state for ρ_i, temperature-enthalpy relations, heat-transfer relations, inter-phase friction correlations, etc. The partial differential equations and the auxiliary relations are also supplemented by appropriate initial and boundary conditions, that express the particular situation to be studied.

3. The Numerical Model

"Finite-domain" equations are formulated by integrating the partial differential equations over control volumes of finite size that taken together fully cover the entire domain of interest (Fig 1). These control volumes (or "cells") are topologically Cartesian, e.g., they can be either strictly Cartesian, or polar cylindrical or generally curvilinear (orthogonal or non-orthogonal), but will always have six sides and eight corners, in the three-dimensional case. For the variables r_i, h_i, m_{il}, p these control volumes are the ones centred on grid nodes such as *P* (in Fig. 1) and having faces which bisect the lines joining *P* to *N*, *S*, *E*, *W* etc. For the velocity componentsu_i, v_i, w_i, the control volumes are displaced in the directions *x*, *y*, or *z*, respectively, by distances which place the relevant velocity locations in their centres. This practice is conventional [1,10,13].

4. Solution Procedure

The equations are both non-linear and strongly coupled, necessitating an iterative solution procedure. There are several such procedures for single-phase flows. An early publication described

the MAC procedure [14], which has subsequently been refined [15,16,19]. The SIMPLE procedure of [1] combined some of the features of MAC with new ones and was also subsequently refined into SIMPLER [12,13] and SIMPLEST [12, 17].

An extension of SIMPLE (and SIMPLEST) to multiphase flows is IPSA (Inter-Phase Slip Algorithm) [13,14,18], a version of which is used for the present work. The algorithm has features in common with a procedure emanating from Los Alamos [19] .

5. Model of Turbulence and Radiation

For the problems under consideration, turbulence and radiation are important and must be modeled appropriately. Below, models are presented that are currently considered as adequate. The interested reader is referred to the appropriate literature for further details and different models.

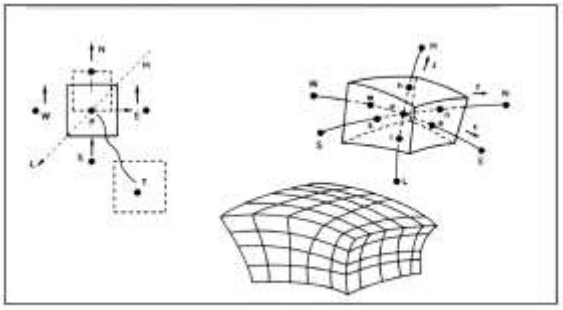

Figure 1. The control volume (topologically Cartesian).

The Radiation Model

The basis of all methods for the solution of radiation problems is the radiative transfer equation (RTE):

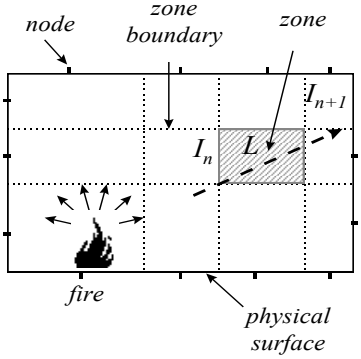

Fig.2: Sub-division of the solution domain into zones

$$\underline{s}\cdot\nabla I(\underline{r},\underline{s}) = -\kappa(\underline{r})I(\underline{r},\underline{s}) + Q(\underline{r},\underline{s}) \qquad (15)$$

which describes the radiative intensity field, I, within the domain, as a function of location vector $(\underline{r})$ and direction vector $(\underline{s})$; Q represents the total attenuation of the radiative intensity due to the gas emission and to the in-scattered energy from other directions to the direction of propagation, and κ is the total extinction coefficient.

The Discrete Transfer Model

The discrete transfer model we use discretizes the RTE along rays. The path along a ray is discretized by using the sections formed from breaking the path at zone boundaries (Fig.2). Details may be found in [20,21,33,34].

Turbulence Description

Turbulence modeling requires models to close the unknown Reynold stresses in the Favre-averaged Navier-Stokes equations, Eqns. (7). These turbulence models have to take into account various interactions. Most numerical simulations of practical systems are based on standard k-ε turbulence models, where transport equations are cast in terms or Favre averages, without explicit combustion effects, which may be important in environmental problems. It appears that refinements in turbulence description could be an important step to improve numerical simulations of turbulent reacting flows. For the computations presented in this work the Renormalization Group model, the RNG k~ε model [22], has been used.

6. Examples of Applications

6.1 Marine Pollution

Prediction of the behavior of oil spills at sea is of crucial importance for impact assessment studies, as the effects of oil toxicity on the marine ecosystem create major environmental problems. The impact of oil toxicity on marine organisms depends on the organism itself and its age, on oil concentration, on the water salinity, its temperature and pH, and on the presence of nutrients, pollutants (sulphides, phenols, detergents) and/or dispersants. Furthermore, the shore damage will also depend on the contact

duration of the slick with the coastline [26-28]. The model described in this paper can account for the above considerations and can therefore predict the environmental impact of an oil-spill. The model considers that the motion of the spill at sea is three-dimensional, transient, and turbulent. The flow is considered as being a two-phase one, the spill and the sea water being the two phases, each characterized by different properties (velocities, densities, etc.).

The model capabilities are demonstrated by applying it to two regions of different topography and bathymetry. These two regions are near Carava (Figure 3), at the island of Lesvos, and near Eretria, in the Evvoikos bay, both being in the Aegean Sea. The first region has a surface of 12x9.5 km^2 and a maximum depth of 55m, whereas the second occupies an area of 10x18 km^2 and has a maximum depth of 25 m.

Figure 3. The region of Carava area

The fate of hypothetical oil spills in the sea was simulated, under transient, two-phase flow conditions, using salt water and meteorological / oceanographical data for a given period of time (May-June 2004). Figures 4,5 present the hydrodynamic field of Carava area and Evvoikos bay, respectively, as predicted by the present model.

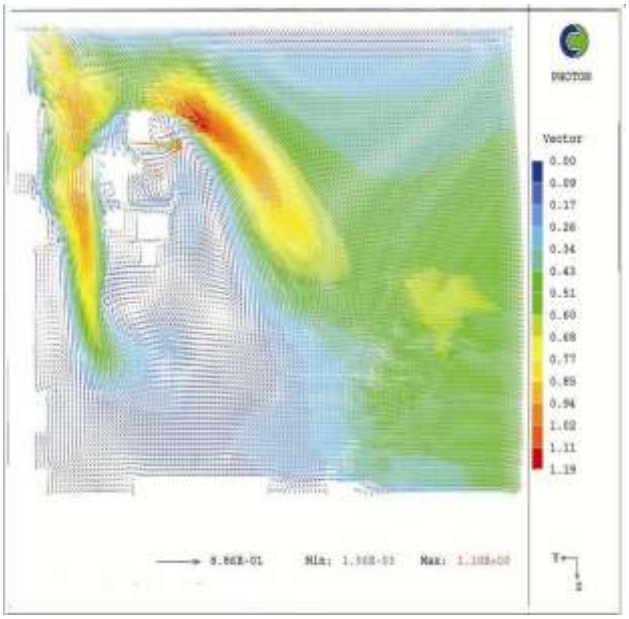

Figure 4. The hydrodynamic field at the surface

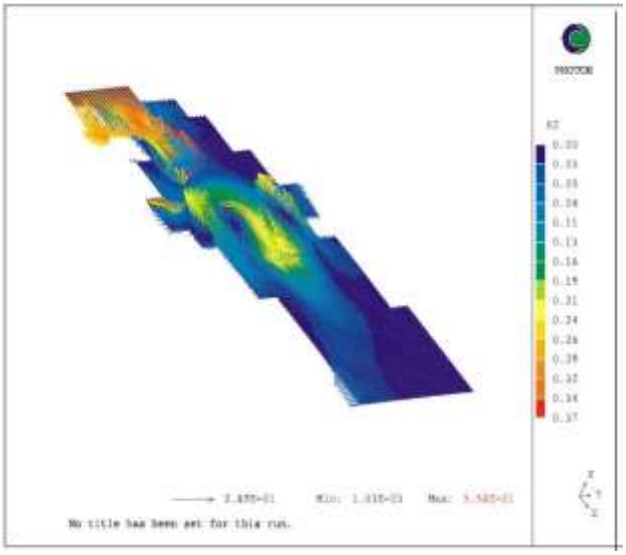

Figure 5. The hydrodynamic field at the surface

Although full runs were performed for both case-studies, space restrictions dictate the presentation of only a few important results. Figure 6 presents the state of an oil spill, a few seconds after a spill of an initial volume of 800 m^3 and a density of 800kg/m^3 took place at a distance of 50 m from the upper eastern coast of the three islands, which are located in the region of Carava, considering a BW wind of 10m/s. Figure 7 presents the fate of the oil spill in the above field 6.5 hours after the accident.

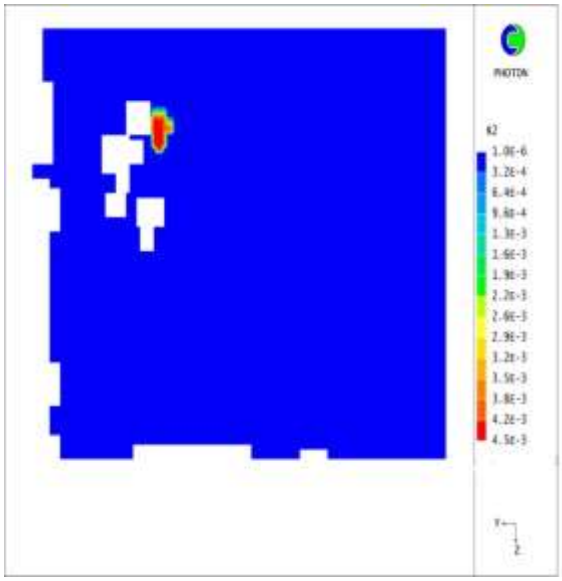

Figure 6. The oil spill 10s after the accident

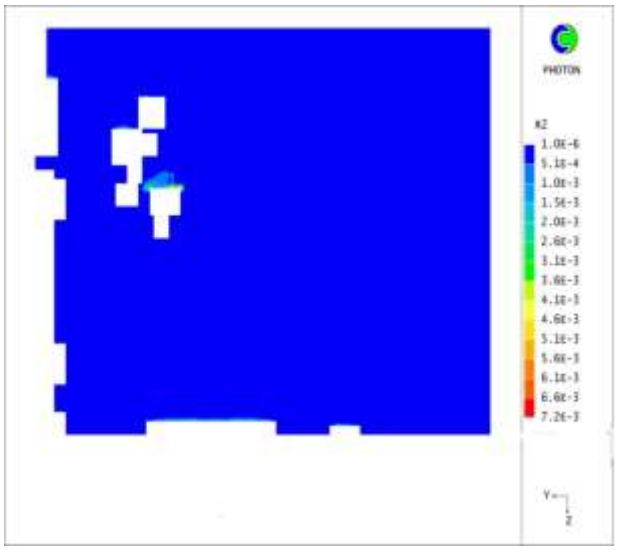

Figure 7. The oil spill 6.5 hours after the accident

Figure 8 presents an oil spill, a few seconds after a discharge of 1000 m^3 of oil of density of 800kg/m^3 had taken place at a distance of 3000 m from the eastern coast of the three islands in the field of Carava area of Lesvos island.

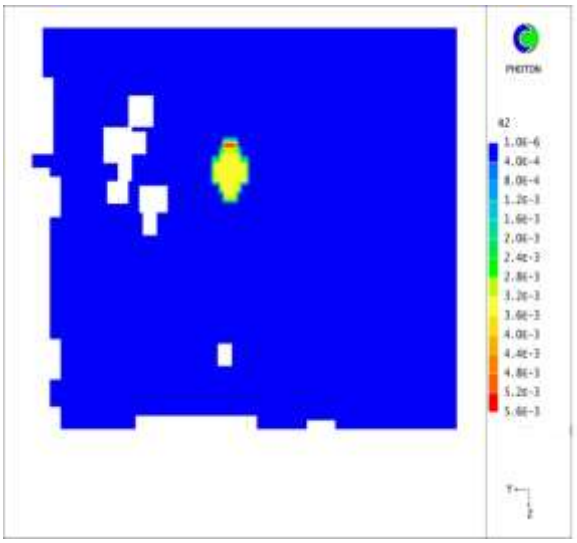

Figure 8. The spill at the surface 10 secs after the accident

Figure 9 presents the spread of the above spill at the surface, 28 days after the accident. It is probable that a break of the spill had happened. Figure 10 presents the spill balance 72 hours after the accident.

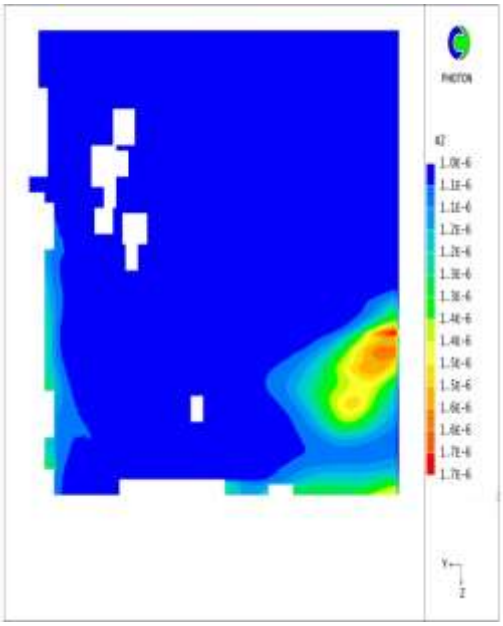

Figure 9. The spill at the surface 28 days after the accident

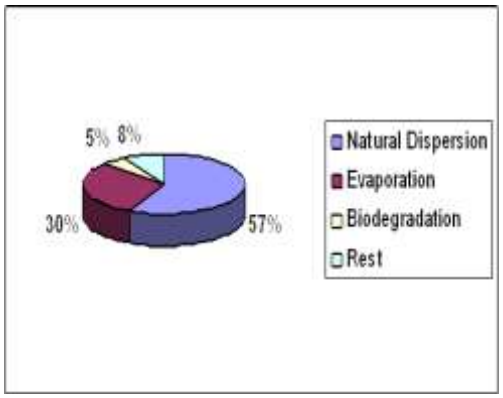

Figure 10: The spill balance 72 hours after the accident

6.2. **Fire Simulations**

Fire may take place in buildings, in industrial complexes, in public transport or in forests. Fire simulations are necessary for designing reliable systems for fire extinction and for the protection of life and property.

The following figures present results of fire simulations. More details may be found in [30-34,39-41].

Fire simulation in a room

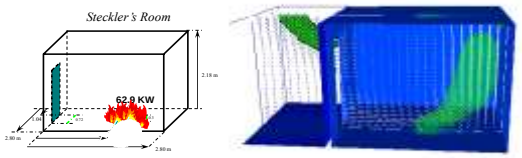

Fig.11. Steckler's Room

Fig. 11 presents the flow during a fire of 62.9 kw strength in Steckler's Room, which is a standard test facility in the USA, used to validate numerical prediction tools.

Fig. 12 presents the comparison of experimental measurements with computer predictions. It is shown that agreement is fair.

Fire simulation - Results

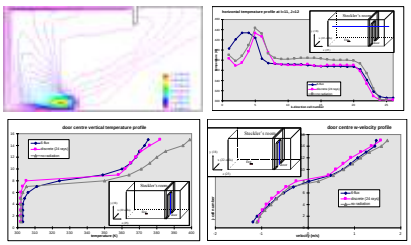

Fig. 12: Steckler's Room. Comparison of predictions with experimental data.

Fig. 13 presents the transient development of fire in the cargo compartment of an airplane and the performance of a water mist system for its extinction. The figure presents temperature contours at 6, 8, 10, 12, 15 and 20 seconds after the fire initiation. Fig. 14 presents the same information at t= 30, 40, 60, 80, 100 and 140 seconds.

Figure 15 presents the effects of ejecting an inert gas for the extinction of the fire at the same cargo compartment. The benefit of using fire simulation tools is now obvious, as it allows engineers and designers to decide on the most efficient type of fire extinction, in order to be fast, safe, practical and not to create toxic by-products.

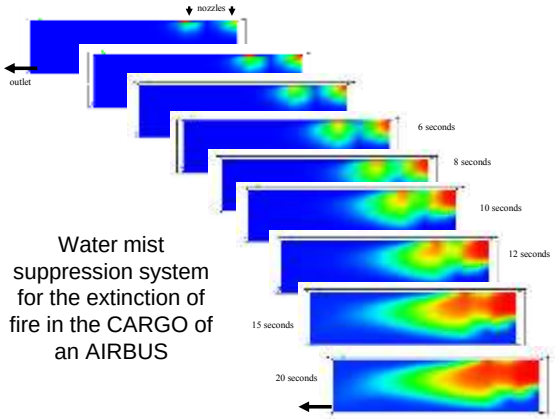

Figure 13: Temperature contours in time

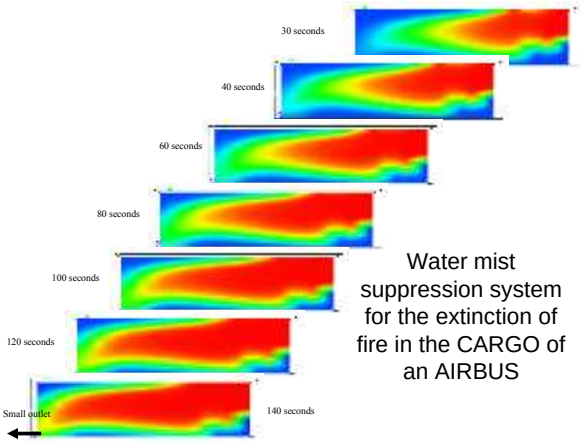

Fig.14: Temperature contours in time.

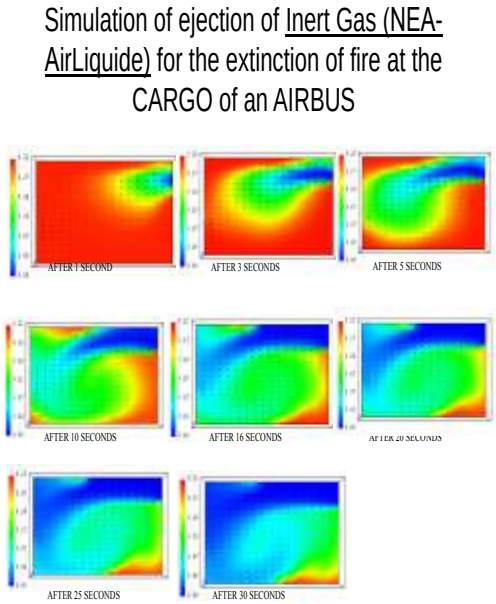

Figure 15: Temperature contours in time.

6.3. Atmospheric pollution

6.3.1 Street Canyons in Cities

Figures 16 and 17 present results that refer to atmospheric pollution. The case is that of a street canyon, i.e. the canyon formed between high buildings in a city (seen on the right and on the left in figs. 16 and 17). The results show that there are cases of recirculation in the canyons. The practical effect of that fact is that, while there may be windy above the buildings and somebody may think that the atmosphere is clear at certain time, pollutants may have been trapped in the street canyon from previous days, and therefore at the height of a walking human the atmosphere is still polluted.

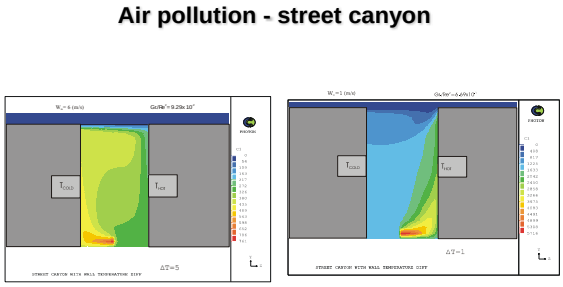

Figure 16 Temperature fields for two sets of conditions

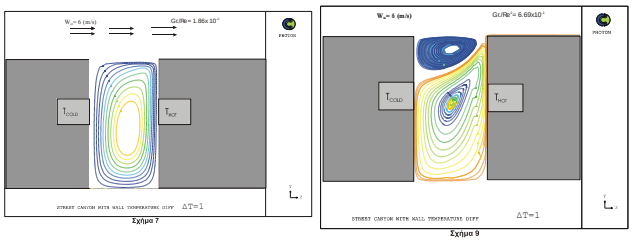

Fig. 17: Flow fields for two sets of conditions

6.4 Toxic pollutants dispersion from large tank fires.

Petrochemical industries normally use large storage tanks, which contain large amounts of flammable and hazardous chemicals. Hence, the occurrence of a tank accident is possible and it usually leads to fire and explosions. Experience has shown that the continuous dispersion of toxic pollutants from large tank fires, such as smoke, SO_2 and CO is responsible for potential environmental and health problems.

Industrial accidents such as that of February 24, 1986, in Thessaloniki, Greece, and the relatively recent large industrial accident of

December 11, 2005, at Oil Storage Depots (Buncefield, Hertfordshire, England) demonstrated unanticipated consequences. The latter one produced a massive fire which engulfed over 20 large fuel - storage tanks. The continuous generation of smoke from these fires presents a potential environmental and health problem that is difficult to assess. In order to try and manage it, it is important to be able to estimate the concentration of the fire-plume pollutants over a wide range of conditions.

The purpose of the presented results is to estimate the dispersion of combustion products and the consequences to the environment from large hydrocarbon - tank fires, as well as the height of the toxic plume (plume rise), and it is from the work by Argyropoulos et al [41]. See also [35,40]. Furthermore, the risk zones for the first respondents, the fire fighters, are identified, by comparing the ground - level concentration of the pollutants with the safety limits. A MUSCL Scheme [42] with deferred correction for the convective terms in the momentum equations, and the CUPID scheme [43] for the convective terms in the scalar conservation equations, were employed to discretize the equations and the solution was obtained using the iterative SIMPLEST algorithm of Spalding [10,11]. The RNG k~ε model [22] was employed with the buoyancy modifications of Markatos et al [30,31], for the modeling of turbulence. Radiation is accounted for by the discrete transfer model described earlier.

For the numerical simulation of the toxic contaminant's dispersion and of the plume rise, an external floating - roof tank has been selected, with dimensions of 85 m diameter and of 20 m height. The tank is surrounded by bunds of 4 m height and 0.5 m width. The geometry of the tank with the bund is illustrated in Figure 18. This type of tank is characterized by the ability of the roof to rise and fall on the stored - fuel surface, according to the latter level, with a maximum storage capacity of 113,432 m^3. Numerical simulations were performed with the use of CFD techniques for a physical domain of 20000 m length (Z-axis), 2200 m width (X-axis) and 2500 m height (Y-axis). These dimensions were chosen following a parametric study, in order to evaluate the extent of the domain after which no major change of the variables was computed close to the tank. Z-axis is the parallel to the wind direction axis, X-axis is the vertical to the wind direction on the ground level axis, while Y-axis is the vertical axis. The tank is situated 543 m from the origin of the Z-axis and 1100 m from the X-axis (symmetry).

Parametric analysis is performed for eight scenarios, all for an adiabatic atmosphere: for two different fuels with heat release rates of 1 and 1.3 MW/m^2, and for four values of wind velocity, 7,8,9 and 11 m/s. We present four of them here, Table 1.

Table 1: Accident scenarios with plume rise estimation.

Scenarios	Fuel	HRR(MW/m^2)	Wind Velocity (m/s)	Plume rise (m)
(1)	Crude Oil	1	8	1746
(2)	Crude Oil	1	11	1335
(3)	Diesel	1.3	8	1781
(4)	Diesel	1.3	11	1417

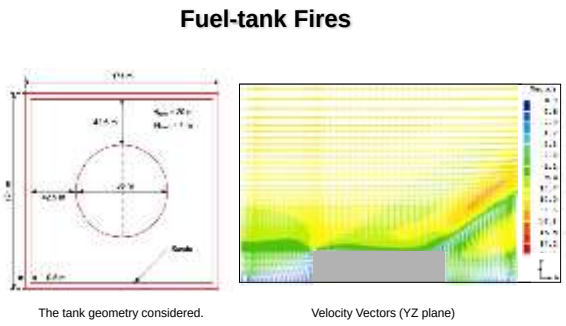

Fig.18: Geometry considered and velocity vectors at a YZ plane.

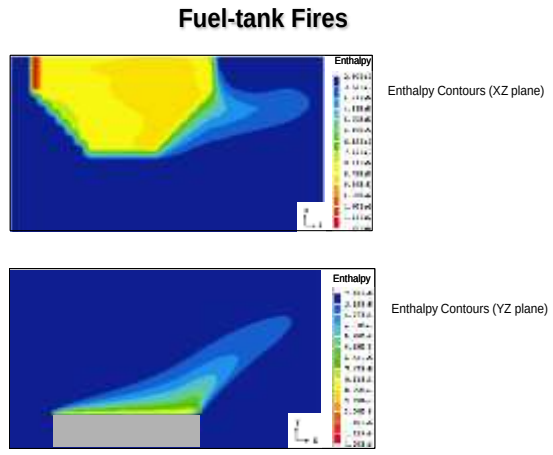

Fig.19: Enthalpy contours at a XZ and at a YZ plane.

Moreover, figs. 20 illustrate concentration of Smoke, CO and SO_2 vs. the height at a position of 5 km from the flow axis.

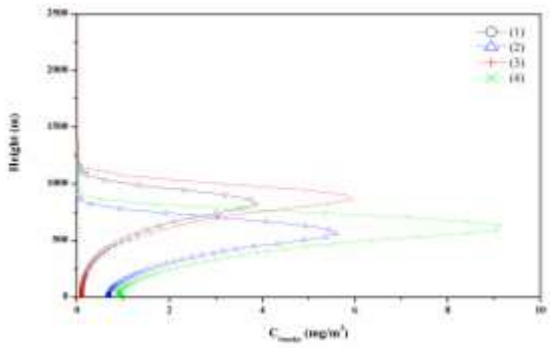

Figure 20 a: Concentration of Smoke vs. the height at a position of 5 km from the flow axis.

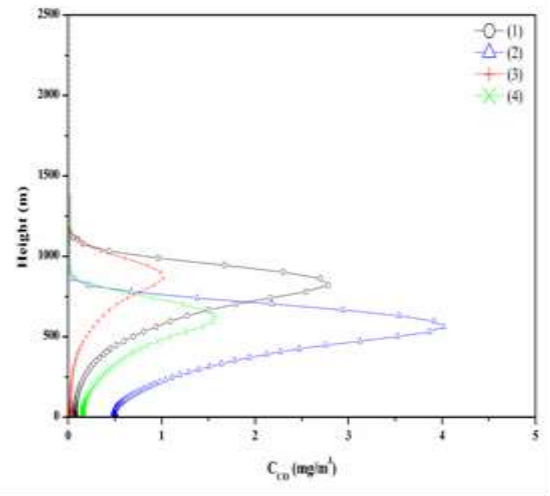

Figure 20 b: Concentration of CO vs. the height at a position of 5 km from the flow axis.

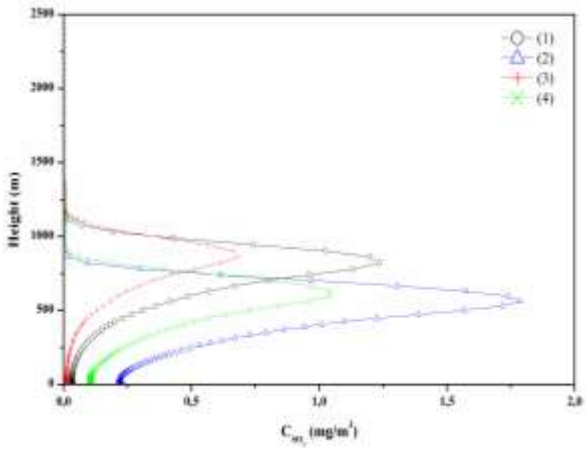

Figure 20 c: Concentration of SO_2 vs. the height at a position of 5 km from the flow axis.

It is observed that for low heights the concentrations of Smoke, CO and SO_2 are extremely high at a position 5 km downwind of the flow axis. On the contrary, with the increase of height the concentrations of Smoke, CO and SO_2 decrease. It is noticed that for heights in the range of 500 – 750 m above the ground level, the value of maximum concentration of Smoke is 9 mg/m^3. Thus, scenario (4) presents the maximum value of Smoke concentration. The lowest value of Smoke concentration is observed for scenario (1) and it is equal to 4 mg/m^3 at a height of 800 m.

The maximum value for CO concentration is found for scenario (2) and is equal to 4 mg/m^3. On the other hand, the minimum value appears for scenario (3) and it is 1 mg/m^3, approximately. The same behaviour is exhibited

for the concentration of SO_2, the maximum value found for scenario (2) and the minimum value for scenario (3), with values of 1,8 and 0,7 mg/m^3.

Hazard identification analysis is performed with the characterization of risk zones (Fig. 21), by comparing the ground level concentration of the pollutants with the safety limits.

The present methodology for the determination of hazard range can be described by comparing the ground level concentrations of the pollutants (smoke, CO, SO_2) with the Lethal Concentration (LC_1) and Immediately Dangerous to Life and Health (IDLH) values of them. The (LC_1) determines the range of the high-risk zone where only fire fighters are allowed wearing the appropriate gear, and (IDLH) specifies the hazard range for the general population [29]. The values for the above safety limits are adopted from the NIOSH website (http://www.cdc.gov/niosh/homepage.html).
The LC_1 (CO) = 9190.18 mg/m^3 and IDLH (CO) = 1374.23 mg/m^3, for SO_2 LC_1 (SO_2) = 2525.97 mg/m^3 and IDLH (SO_2) = 262 mg/m^3. Limit values for smoke are LC_1 (Smoke) = 25000 mg/m^3 and IDLH (Smoke) = 2500 mg/m^3.

From the parametric runs above, the ground – level concentrations of toxic pollutants for the two zones are computed for all scenarios. According to those data, there are no "death zones" due to the concentrations of Smoke, CO and SO_2. In the first zone the concentrations which are observed are high, especially for smoke, but do not exceed the safety limits of LC_1 or IDLH.

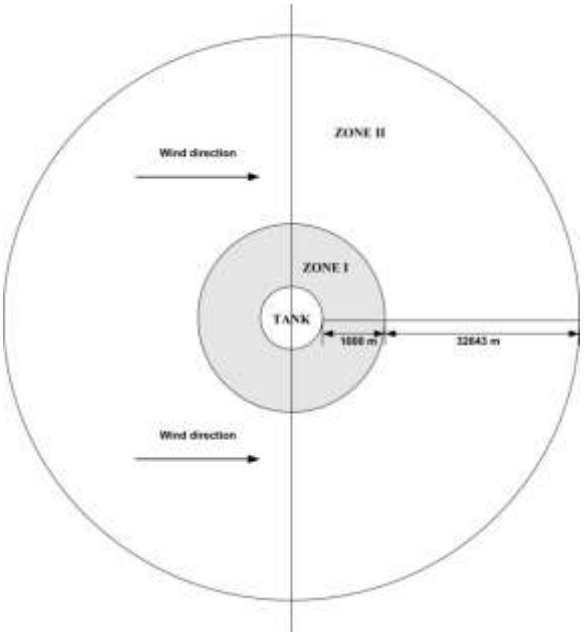

Figure 21: Configuration of risk zones I and II

7. Conclusions

- Methods now exist for computing complex phenomena with a view of protecting the Environment, saving energy and controlling major hazards. These methods can be of great help to the environmental engineer and scientist, for the design of complex environmental-protection systems and for any relevant decision – making process

- 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 assist with the comparisons.

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