Numerical Simulation of the Air Pollutants Dispersion Emitted by CHP Using ANSYS CFX

Oliver Mărunțălu, Gheorghe Lăzăroiu, Elena Elisabeta Manea, Dana Andreya Bondrea, Lăcrămioara Diana Robescu

Abstract—This paper presents the results obtained by numerical simulation using the software ANSYS CFX-CFD for the air pollutants dispersion in the atmosphere coming from the evacuation of combustion gases resulting from the fuel combustion in an electric thermal power plant. The model uses the Navier-Stokes equation to simulate the dispersion of pollutants in the atmosphere. It is considered as important factors in elaboration of simulation the atmospheric conditions (pressure, temperature, wind speed, wind direction), the exhaust velocity of the combustion gases, chimney height and the obstacles (buildings). Using the air quality monitoring stations it is measured the concentrations of main pollutants (SO_2, NOx and PM). The pollutants were monitored over a period of 3 months, after that the average concentration are calculated, which is used by the software. The concentrations are: 8.915 $\mu g/m^3$ (NOx), 9.587 $\mu g/m^3$ (SO_2) and 42 $\mu g/m^3$ (PM). A comparison of test data with simulation results demonstrated that CFX was able to describe the dispersion of the pollutant as well the concentration of this pollutants in the atmosphere.

Keywords—Air pollutants, computational fluid dynamics, dispersion, simulation.

I. INTRODUCTION

THE electric thermal power plant Grozavesti has the main activity to produce electricity and thermal energy, based on the conversion of the chemical energy of the fossil fuel (natural gas and fuel oil). The electricity and most of the heat are produced in cogeneration mode. 99 % of heat produced is distributed as warm water to the main consumer, RADET (Bucharest Autonomous Company for Thermal Energy Distribution) and the electricity produced into the National Energy System, to cover the national consumption. The gases from the fuel combustion processes in the two boilers of the combustion plant are evacuated by chimneys with a maximum height of 60 meters. Combined heat and power (CHP) plant has 100 MW installed electric power and585 Gcal/h thermal energy capacity [1].

The integral models and computational fluids dynamics (CFD) are used for modeling of the pollutants dispersion. Examples of the integrated models are AERMOD, TAPM,

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FARM, CMAQ and many others are widely used because of the ease of use and fast computation time. Using CFD helps to solving fluid flow problems. CFD models can give a detailed description of the physical processes and the complex geometries can be handled.

To perform the pollutant dispersion simulation ANSYS CFX 14.0 is used. The quality of simulation results is influenced by uncertainties or errors of parameters related on the numerical methods and physical models. The air quality in the power plant area is monitored with air quality monitoring station, which measures the concentration of the pollutants (SO_2, NO_2, NOx, O_3, CO, PM_{10}, $PM_{2.5}$ and Pb) within a radius of 5 km. This station measures the meteorological parameters (temperature, wind velocity and direction, relative humidity, atmospheric pressure and solar radiation) which are very important for achieving the simulation. The monitoring station is equipped with sulfur dioxide analyzer (AF 21 M2), carbon monoxide analyzer (CO 11 M2), nitrogen dioxide analyzer (AC 31 M2), ozone analyzer (O3 41 M2) and particulate sampler (LVS Derenda 31./PNS 2.1-15). The methods used to determine the concentration of air pollutants are:
- Ultraviolet fluorescence method (SO_2);
- Chemiluminescence method (NOx);
- Gravimetric method (PM_{10});
- Nondispersive infrared spectrometry method (CO);
- Photometric method (O_3).

II. SIMULATION SETUP WITH ANSYS CFX

ANSYS CFX software is able to solving complex and diverse three-dimensional fluid flow problems. To describe the fundamental processes of momentum, mass transfer and heat, it used the Navier-Stokes equations. The software contains a number of mathematical models that can be used with Navier-Stokes equations to describe other chemical or physical processes, such as combustion, turbulence or radiation. It uses a finite volume approach to convert partial differential equations in a discrete system of algebraic equations by discretizing the computational domain into finite elements. These equations lead to a solution with specified domain boundary conditions. For a transient simulation, initial conditions are also required numerically close the equations. One of the most important features of CFX is that it uses a coupled solution requiring less iteration to achieve convergence solution [2], [3].

For modeling the dispersion of the pollutants in the atmosphere by the thermal power plant chimney with ANSYS CFX five steps are required: creating the geometry, meshing, pre-processing, solving and post-processing. To configure the

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simulation only the first three steps are considered. In Table I all the essential inputs or parameters in the setup process are listed [4].

TABLE I
SUMMARY OF INPUT VARIABLES FOR POLLUTANT DISPERSION SIMULATION SETUP

Components	Parameters
Geometry creation	3D geometry (CHP and obstacles)
Meshing	Mesh shape and size
Pre-processing domain	Fluid properties
	Turbulence model
Pre-processing atmosphere boundary	Fluid compositions
	Wind direction and velocity profile
	Temperature profile
	Turbulence profile
Pre-processing CHP chimney boundary	Fluid composition
	Gases evacuation velocity
	Gases temperature
	Turbulence
Pre-processing ground boundary	Influence
	Surface

A. Creating the Geometry

In a CFD simulation, first step is to create the geometry of the flow field. The flow field of interest is represented by a computational domain within which the equations of fluid flow and heat transfer are solved. When modeling the dispersion of pollutant in atmosphere, we must consider the objects around the pollution source, the obstacles that may encounter the smoke cloud and wind direction. These elements must be constructed in the domain to see the effects on the cloud dispersion. Some geometries can contribute to increasing the concentration of the pollutants by reducing the wind velocity or decreasing the atmospheric turbulence [5].

B. Meshing

The second step in achievement the modeling is dividing the computational domain. The computational domain is discretized into a number of small control volumes, a mesh generated automatically by CFX-Mesh. The mesh had structured grids in the near wall region and unstructured grids in the rest of the domain, which contains prismatic, tetrahedral and pyramidal elements. ANSYS CFX provides a list of criteria for evaluating the quality of the mesh through mesh-associated parameters such as the edge length ratio. Maximum and minimum face angles, connectivity number, element volume ratio, smoothing level, number of retries, mesh morphing [6]. In order to avoid the adverse effect on the simulation accuracy the mesh size must be chosen carefully [7]-[9].

C. Domain and Boundary Conditions

1. Domain

ANSYS CFX is not designed especially as a consequence model for emitted pollutants in the atmosphere hazards, and therefore fluid properties and physical models should be identified to characterize the physical process of pollutants dispersion in the atmosphere when defining the domain.

For the production of energy, the CHP uses fuel oil and natural gas. The molecular composition of the fuel oil varies widely from formation to formation but the proportion of chemical elements varies in narrow limits. The natural gas is manly composed of methane, but may also contain small amounts of ethane, propane, and heavier hydrocarbons [10]. Table II shows the composition of fuels used by the studied CHP. Combustion of fuels leads to production of polluting gases (CO_2, SO_2, N_2, and PM). The combustion is performed in five large combustion installations (LCI1-476 MW, LCI2-LCI5-116 MW) [11].

TABLE II
COMPOSITION OF FUEL OIL AND NATURAL GAS USED FOR COMBUSTION

Components	Fuel oil (%)	Natural gas (%)
Carbon	85.75	-
Hydrogen	9.4	-
Nitrogen	0.2	2.56
Oxygen	1.3	0.02
Sulfur	3.35	-
Minerals	<0.1	-
CH_4	-	85.47
C_2H_6	-	5.73
C_3H_8	-	2.18
CO_2	-	0.27

The emission limit values are determined using:

$$TLV = \frac{\sum TLV_i \cdot Q_i \cdot H_i}{\sum Q_i \cdot H_i} \qquad (1)$$

where, TLV is the threshold limit value, TLV_i is the threshold limit value for the pollutant, Q_i is the fuel flow, H_i is combustion heat of the fuel.

ANSYS CFX offers a wide variety of turbulence models, such as k-ε model, k-ω model, and shear stress transport (SST) model [5]. In this study, the standard k-ε model was used considering both computational time and precision. This model is also used by other authors for numerical simulation of air pollutant dispersion [12], [13].

2. Atmosphere Boundary

The atmospheric surface layer is the region of interest where the pollutants are released. An accurate description of airflow in the atmospheric surface layer is of prime importance to make CFD codes generate reliable simulation results. Almost all atmosphere-related simulations have modeled the airflow in this layer as fully developed horizontally homogeneous, in which the mean variables are only dependent on the height z. In a simulation with ANSYS CFX, the atmospheric boundary is always set as an open boundary, where fluids can simultaneously flow in and out of the domain. Wind velocity, temperature, and turbulence profiles are developed to represent the characteristics of these variables in real situations. In the atmospheric surface layer, the momentum and heat vertical fluxes do not vary by more than 10%. Due to these small flux variations, the use of the Monin–Obukhov similarity theory is recommended to

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describe the wind velocity, temperature, and turbulence profiles [14], [15].

The wind velocity and potential temperature gradient functions along the height z are given as [16].

$$\frac{\partial U}{\partial z} = \frac{U_*}{k \cdot z} \cdot \phi_m \left(\frac{z}{L} \right) \tag{2}$$

$$\frac{\partial \theta}{\partial z} = \frac{\theta_*}{k \cdot z} \cdot \phi_h \left(\frac{z}{L} \right) \tag{3}$$

where L is the Monin-Obukhov length, U_* is the friction velocity, θ_* is the scaling potential temperature and k is the von Karman constant (0.41).

Integrating (2) and (3) from z_0 to z obtain:

$$U(z) = \frac{U_*}{k} \left[ln \left(\frac{z}{z_0} \right) - \psi_m \left(\frac{z}{L} \right) \right] \tag{4}$$

$$\theta(z) = \theta_0 + \frac{\theta_*}{k} \left[ln \left(\frac{z}{z_0} \right) - \psi_h \left(\frac{z}{L} \right) \right] \tag{5}$$

where

$$\psi_m \left(\frac{z}{L} \right) = \int_{z_0}^{z} \left(\frac{1}{z} - \frac{\phi_m(z/L)}{z} \right) dz \tag{6}$$

$$\psi_h \left(\frac{z}{L} \right) = \int_{z_0}^{z} \left(\frac{1}{z} - \frac{\phi_h(z/L)}{z} \right) dz \tag{7}$$

where z_0 is the surface roughness height and θ_0 is the potential temperature at z_0.

The potential temperature is related to the ambient temperature and pressure by

$$\theta = T \left(\frac{P_0}{P} \right)^{\mu} \tag{8}$$

where T is the actual temperature, P is the actual pressure, P_0 is the standard reference pressure, and μ=0.285. The potential and actual temperatures in the atmospheric surface layer, in absolute units, do not differ by more than 10% [17].

In the Cartesian system the components of the wind velocity in three directions are then expressed by introducing the wind direction angle α:

$$U_x(z) = U(z) \cdot \cos(\alpha) \tag{9}$$

$$U_y(z) = U(z) \cdot \sin(\alpha) \tag{10}$$

$$U_z(z) = 0 \tag{11}$$

ANSYS CFX cannot automatically calculate the turbulence characteristics, such as turbulence kinetic energy k and eddy dissipation rate ε. One approach to deal with this limitation is to relate these variables to the Monin-Obukhov length [18]:

$$k(z) = 5.48 U_*^2 \sqrt{\left[\frac{\phi_m z/L}{\phi_h z/L} \right]} \tag{12}$$

$$\varepsilon(z) = \frac{U_*^3}{k \cdot z} \phi_h \left(\frac{z}{L} \right) \tag{13}$$

The functions ϕ_m (z/L), ϕ_h (z/L), ψ_m (z/L), ψ_h (z/L) can be expressed as empirical relations with the Monin-Obukhov [19]:

When L>0:

$$\phi_m \left(\frac{z}{L} \right) = \phi_h \left(\frac{z}{L} \right) \tag{14}$$

$$\psi_m \left(\frac{z}{L} \right) = \psi_h \left(\frac{z}{L} \right) \tag{15}$$

When L<0:

$$\phi_m \left(\frac{z}{L} \right) = \frac{1}{x} \tag{16}$$

$$\phi_h \left(\frac{z}{L} \right) = \frac{1}{x^2} \tag{17}$$

$$\psi_m \left(\frac{z}{L} \right) = 2ln \left(\frac{1+x}{2} \right) + ln \left(\frac{1+x^2}{2} \right) - 2tan^{-1}(x) + \frac{\pi}{2} \tag{18}$$

$$\psi_h \left(\frac{z}{L} \right) = 2ln \left(\frac{1+x^2}{2} \right) \tag{19}$$

with

$$x = \sqrt[4]{\left(1 - \frac{16z}{L} \right)} \tag{20}$$

To solve these equations, the wind velocity and temperature must be measured at least for two different heights. Another alternative approach to represent the wind velocity and turbulence profiles associated with the k-ε turbulence model if measurements are made at only one height is proposed as [20]:

$$U = \frac{U_*}{k} ln \left(\frac{z+z_0}{z_0} \right) \tag{21}$$

$$k = \frac{U_*^2}{\sqrt{C_\mu}} \tag{22}$$

$$\varepsilon = \frac{U_*^3}{k(z+z_0)} \tag{23}$$

where c_μ is the turbulence constant (0.09).

Using this method, the temperature is assumed constant along the height z.

3. Chimney

The chimney can be specified as inlet boundary, where the pollutants are emitted into the domain. The essential parameters to describe the chimney boundary are the concentration of pollutants, the stack height, the exhaust velocity and the gases temperature.

First combustion installation with a power of 476 MW is equipped with a reduced NOx burner formation and an exhaust chimney with a height of 60 m and a diameter of 4.2 m. The other four combustion installations, with a power of 116 MW each, are each equipped with one chimney, with a height of 55 m and a diameter of 3.2 m. The emitted pollutants are SO_2, NOx, and PM [21], [22].

The calculation of the fuel gases volume and the concentration of pollutants are as [23].

$$V_{CO_2} = 0.01867 \cdot C \tag{24}$$

$$V_{SO_2} = 0.00700125 \cdot S \tag{25}$$

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$$V_{N_2} = 0.79 \cdot V_{a\ min} + 0.08 \cdot N \qquad (26)$$

where $V_{a\ min}$ is the stoichiometric volume of air used for combustion. The volumes are measured in m^3/kg.

The stoichiometric volume of fuel gases is calculated by summing the components of the fuel gases.

$$V_g = V_{CO_2} + V_{SO_2} + V_{N_2} \qquad (27)$$

$$c_{SO_2} = \frac{m_{SO_2}}{V_g} \cdot 10^6 \qquad (28)$$

$$c_{NO_x} = \frac{m_{NO_x}}{V_g} \cdot 10^3 \qquad (29)$$

$$c_{ash} = \frac{m_{ash}}{V_g} \cdot 10^3 \qquad (30)$$

where c_{so2}, c_{NOx} and c_{ash} are the concentration for SO_2, NO_x and ash; m_{SO2}, m_{NOx} and m_{ash} are the mass of SO_2, NO_2 and ash.

4. Initial Conditions

The gases composition, height-dependent wind speed, ambient temperature, turbulence kinetic energy, and energy dissipation rate must be specified throughout the domain as initial conditions. These initial values are set close to values in the atmospheric boundary to create an initial state with only wind flow through the domain and no polluting gases.

III. ANSYS CFX SIMULATION

The computational domain where de simulation is performed is considered a box with dimensions 200x150x100 m. The specification of the domain can be seen in Table III. The CHP is located in a populated area that created discomfort by the emitted smoke which containing pollutants, and noise. Figs. 1 and 2 represent the location of the CHP and geometric construction for simulation. Only one chimney was considered for simulation, namely the one of the combustion installation with power of 476 MW.
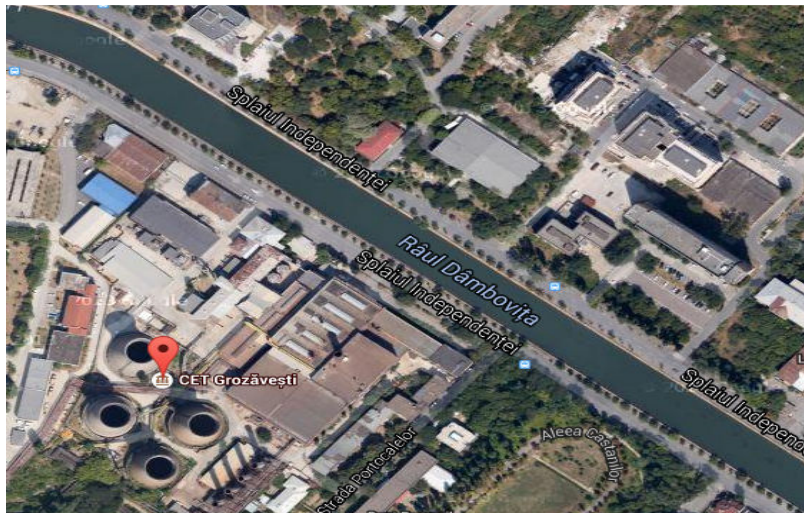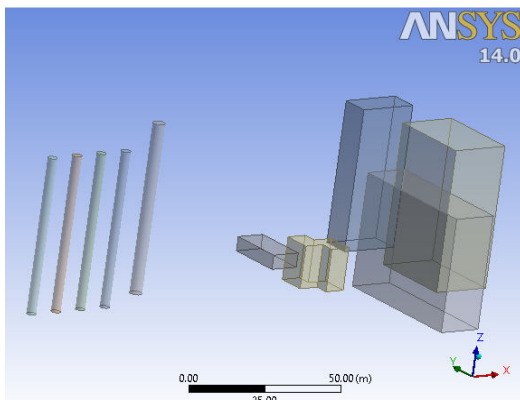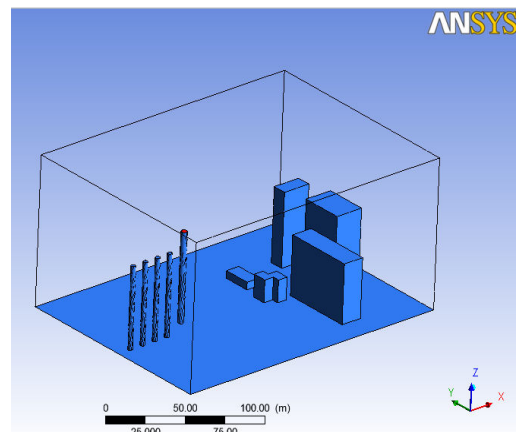

Fig. 1 Satellite view of the location [24]

(a)

(b)

Fig. 2 (a) The geometry inside of the domain; (b) Wireframe

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TABLE III
SPECIFICATION OF THE DOMAIN

Object	Dimensions (m)
Chimney 1	60
Chimney 2	55
Chimney 3	55
Chimney 4	55
Chimney 5	55
Building 1	7x10x15 p
Building 2	15x50x40
Building 3	20x30x50
Building 4	10x20x5
Building 5	20x30x50

physics [25], [26].

TABLE IV
THE MESHING SETTINGS

Relevance center	Fine
Smoothing	High
transition	Fast
Span Angle Center	Coarse
Body Sizing	250 mm
Minimum Edge Length	5 m
Triangle Surface Mesher	Program Controlled
Physics Preference	Mechanical
Rigid Body Behavior	Dimensionally Reduced

Fig. 3 depicts the meshing detail of the geometry. The entire domain was mainly composed of tetrahedral cells, with a small amount of prism and pyramid cells in the inflation layers to better model the close to wall physics of the flow field such as the velocity gradient. The settings for the mesh are presented in Table IV.

All simulation were carried on a laptop using an Intel Core i5-4200H, 2800MHz CPU, 8 GB of RAM and video card GeForce GTX 850M 2GB.
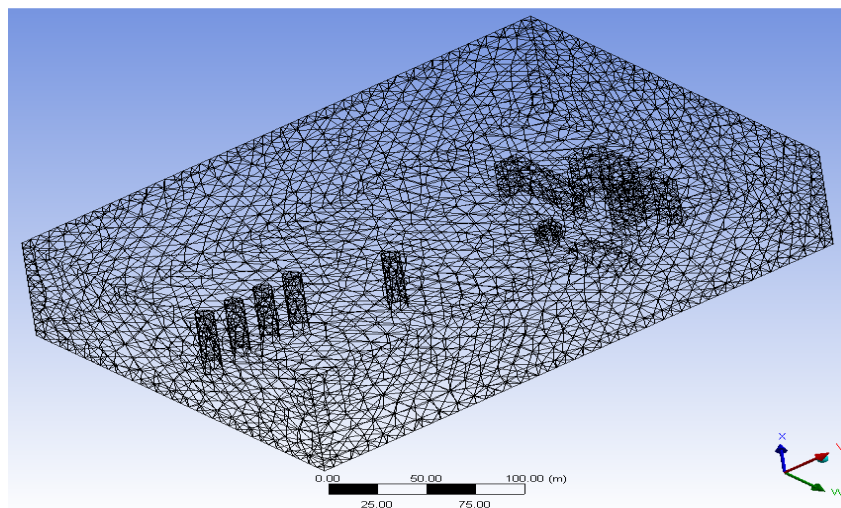
IV. RESULTS AND DISCUSSION

The results are presented in Fig. 4. Mesh size is a key parameter in controlling spatial discretization, which is associated with truncation error of Taylor series in the numerical method when calculating flow variable gradient at the face of a control volume [4].
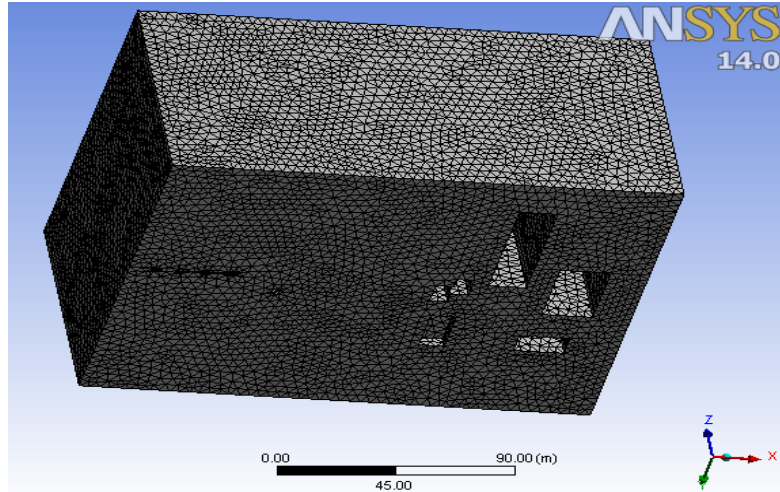
Uncertainties in CFD simulation results arise from different sources, which can be generally numerical errors and uncertainties and errors and uncertainties in modeling the

The simulation parameters for these results are the wind velocity, exhaust velocity and total concentration of smoke pollutants. The exhaust velocity was v_g=0.1 m/s, the wind velocity v_w=1 m/s (considered a day without turbulence) and the N-S direction is chosen for the wind because there is the nearest inhabited area. Fig. 4 shows the evolution of the smoke cloud. Other results of the simulation are presented in Fig. 5. It can be observed the velocity and pressure distribution in the computational domain.

The behavior of the plume is affected by a number of parameters, including the initial source conditions (exit velocity and difference between the plume temperature and that of the air), the stratification of the atmosphere, and the wind velocity. Characterization of plume rise in terms of the exhaust gas properties and the ambient atmospheric state is a complex problem. The most detailed approach involves solving the coupled mass, momentum, and energy conservation equations. This approach is generally not used in routine calculations because of its complexity.
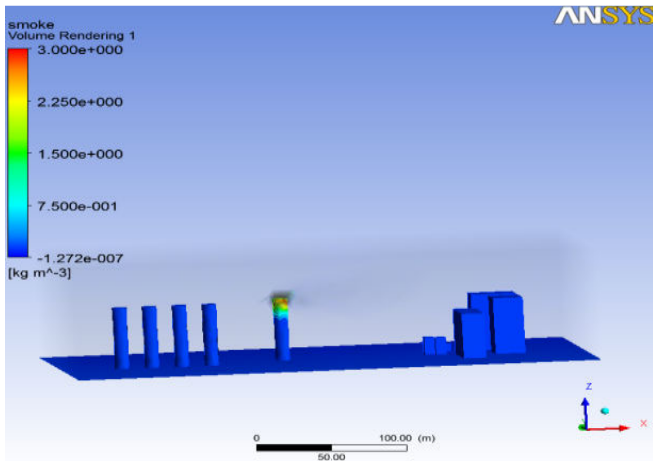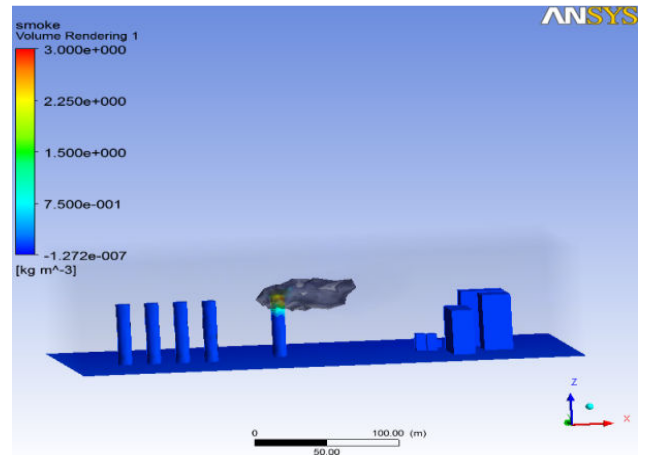

(a)

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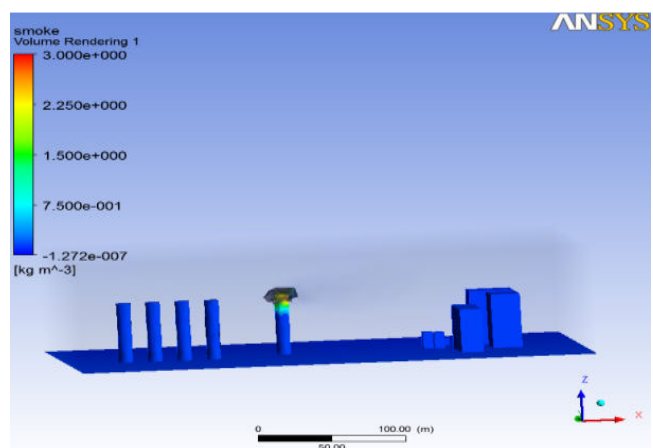Vol:9, No:9, 2015

(b)

Fig. 3 (a) Internal surfaces meshing; (b) Final meshing detail

(a)
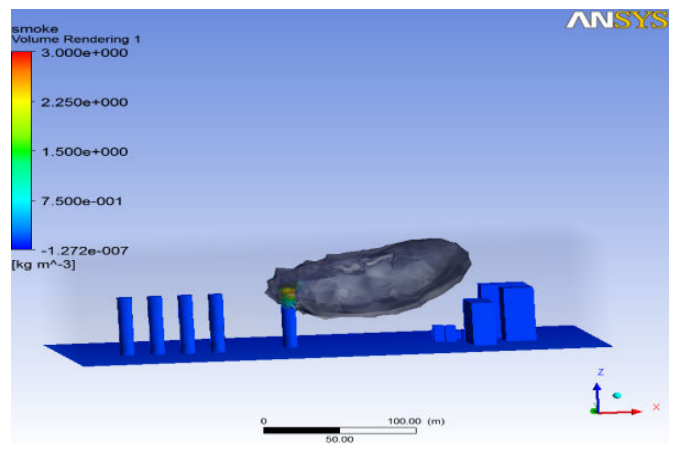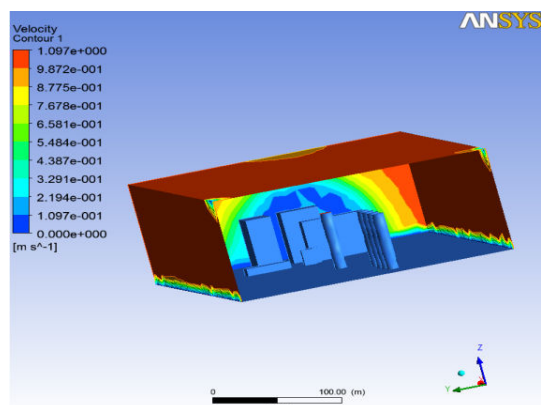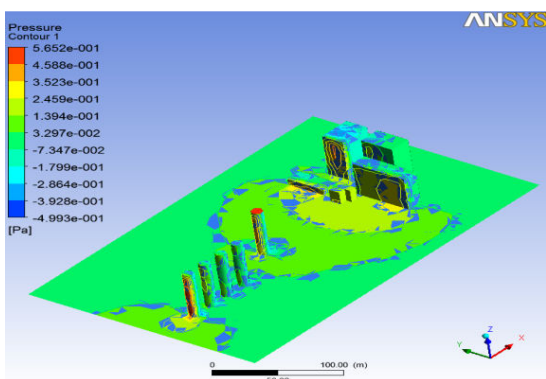

(c)

(b)

(d)

Fig. 4 Plume evolution in time: (a) 5s; (b) 30s; (c) 75s; (d) 120s

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(a)

(b)

Fig. 5 (a) Velocity distribution; (b) Pressure distribution

V. CONCLUSION

ANSYS CFX-CFD is used to investigate the dispersion of the pollutants emitted by CHP, which uses fossil fuels to produce energy. This software is able to describe the dispersion of the pollutant as well the concentration of this pollutants in the atmosphere. The essential parameters to setup a CFD simulation are identified.

The exhaust smoke has the form of the Gaussian plume.

To get results in less time a performing system is required to reduce the computing time.

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