Aerosol and Air Quality Research, 11: 758–762, 2011
Copyright © Taiwan Association for Aerosol Research
ISSN: 1680-8584 print / 2071-1409 online
doi: 10.4209/aaqr.2010.11.0092

A CFD Simulation Study of VOC and Formaldehyde Indoor Air Pollution Dispersion in an Apartment as Part of an Indoor Pollution Management Plan

Ioannis K. Panagopoulos[1*], Athanasios N. Karayannis[1], Pavlos Kassomenos[2], Kostantinos Aravossis[3]

[1] *Sybilla ltd., 16 Ypsilandou st., Maroussi 151 22, Athens, Greece*
[2] *Department of Physics, University of Ioannina, University Campus 45 110, Ioannina, Greece*
[3] *Sector of Industrial Engineering and Operational Research, School of Mechanical Engineering, National Technical University of Athens, Polytechnioupolis, Zografos 174 54, Athens, Greece*

ABSTRACT

This paper is a preliminary report of an indoor pollution case study in a complex of apartments as a part of an Indoor Pollution Management Plan (IPMP). It describes the calculation by Computational Fluid Dynamics (CFD) techniques and presents the predicted air flow, Volatile Organic Compounds (VOCs) and formaldehyde contaminant distributions in an apartment comprised of a full-scale kitchen with open access to a living room, ventilated by an exhaust hood. The CFD Code PHOENICS®, which is based on solving the full 3-D Navier Stokes equations for turbulent flow and scalar conservation equations, was used. Major kitchen indoor pollution sources, VOCs and formaldehyde emitting materials and their emission characteristics were calculated through the use of emission factors. A typical apartment was used under case study and its detailed geometry was applied for the CFD model. To analyze the characteristics of the indoor environment, different mixing ventilation schemes (different locations of the cooker/oven and air inlets) were chosen as the parameters to investigate the indoor environment. The fields of VOCs and formaldehyde for several air inlets window positions, and ventilation parameters were calculated and compared. It was concluded that CFD methods can be used as a useful tool to assist the rational design of indoor spaces.

Keywords: CDF; Indoor air pollution; Numerical modelling; Turbulence; Indoor sources.

INTRODUCTION

Indoor air quality is a major concern for businesses, and building managers, tenants, and employees because it can impact the health, comfort, well being, and productivity of the building occupants. Most Europeans and Americans spend up to 90% of their time indoors and many spend most of their working hours in an office environment. Studies conducted by the U.S. Environmental Protection Agency (USA/EPA, 1997) and others conclude that indoor environments may sometimes show levels of pollutants that are actually higher than levels found outside (USA/EPA, 1997). Pollutants in an indoor environment can increase the risk of illness. Several studies by USA/EPA, states, and independent scientific panels have consistently ranked indoor air pollution as an important environmental health problem quality (USA/EPA, 1995; USA/EPA, 1997). While most buildings do not have severe indoor air quality problems, even well-managed buildings can sometimes experience episodes of poor indoor air quality (USA/EPA, 1997; Environment Australia, 2001).

Volatile Organic Compounds (VOCs) constitute an important class of indoor air contaminants. Evidence from a variety of non-industrial building investigations and systematic studies found that 60% of VOCs indoor emissions come from building material and furnishings (De Bellie *et al*., 1997; Toxics and Interior Finishes Healthy Building Networks, 2006). Various VOCs have been associated with certain symptoms of "sick building syndrome" and multiple chemical sensitivity, and other health effects (USA/EPA, 1991; CBS, 1995).

The emission of formaldehyde from building materials has long been recognized as a significant source of the elevated concentrations of formaldehyde frequently measured in the indoor air. Pressed wood products (i.e., particleboard, MDF and hardwood plywood) are now considered the major sources of residential formaldehyde contamination (Godish, 1988). Pressed wood products are bonded with urea-formaldehyde (UF) resin; it is this adhesive portion that is responsible for the emission of formaldehyde into

---

[*] Corresponding author. Tel.: +30 210 8024244;
Fax: +30 210 6141245
E-mail address: j.k.panagopoulos@sybilla.gr

indoor air. Generally, the release of formaldehyde is highest from newly made wood products. Emissions then decrease over time, to very low rates, after a period of years (Godish, 1988). Concentrations of formaldehyde in indoor air are primarily determined by source factors that include source strength, loading factors and the presence of source combinations (Godish, 1980). Relatively high concentration levels of formaldehyde are found in outdoor urban environment as well (Wang *et al*, 2010).

Indoor Air Quality Computer models (IAQ computer models) have been developed and increasingly used for predicting indoor air pollutant concentrations. Five principal factors controlling the generation and ultimate fate of an emission in a room with restricted flow have been identified: sources, sorption/desorption, mixing volume, air exchange, and removal. In order to account for these factors especially for the possible non-uniform VOC distributions in buildings, certain models based on Computational Fluid Dynamics-CFD techniques have also been developed. The CFD-based IAQ models solve a set of conservation equations describing the flow, energy, and contaminants in the system.

This work attempted to develop a CFD-based model for general Indoor Air Quality studies adopting conservative contaminant emissions factors. The CFD model integrated the effects of airflow and turbulent characteristics associated VOC and formaldehyde emission sources to yield the detailed distributions of airflow, temperature, and contaminant in buildings. Such knowledge is needed by engineers and architects for selecting appropriate ventilation systems and control strategies to minimize indoor contaminant exposures. IAQ model (and CFD models) can contribute in the successful implementation of these strategies, leading to an IPMP consisting of guidance (or relative procedures) for operation timing and relative flow-rate of the ventilation system combined with simple activities like opening the windows for certain amount of time each day. Use of the model is demonstrated by applying it to study IAQ in a room with three different mixing ventilation schemes, and by analyzing the characteristics of air flow and contaminant distribution in a full-scale kitchen with open access to a living room, ventilated by an exhaust hood. Kitchen and gas cooking activities are, also, a significant source of air pollutants and airborne particles indoors (See and Batasubramanian, 2006).

THE PHYSICAL PROBLEM CONSIDERED

Fig. 1 presents the plan view of an apartment with a floor area of 98 m^2. Details of the living room and kitchen arrangement are presented in Fig. 2. LNG gas was used as fuel. The relevant kitchen hood (opening gas range) dimensions were 0.3 m × 0.3 m × 0.1 m.

In this study different air inlets (window-Scenario A, hole 1-Scenario B and hole 2-Scenario C as shown in Fig. 2), corresponding to different air pattern distributions and mixing schemes, were chosen as parameters to investigate the indoor environment, while the overall ventilation rate was set constant in compliance with California/USA regulations (CCR, 2001) and ASHRAE Standards 62.2-2003 (ASHRAE, 2001) (see paragraph 3.2.2 below).

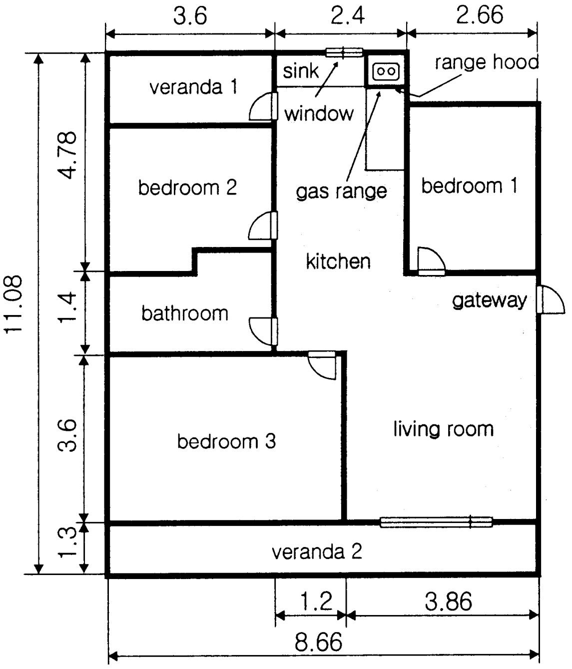

Fig. 1. Plane view of a model apartment. [unit; m].

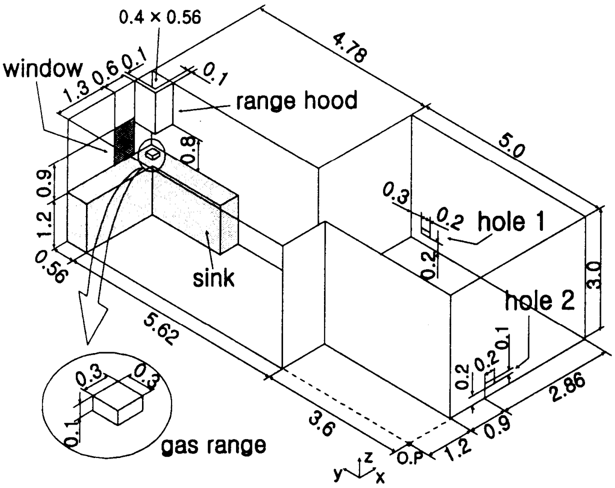

Fig. 2. Schematic diagram of the kitchen and living room.

CALCULATIONS PERFORMED

Numerical Model Description

PHOENICS (CHAM, 2002) is a general purpose software package which predicts quantitatively how fluids (air, water, oil, etc) flow in and around engines, process equipment, buildings, natural-environment features, and so on. It also calculates the associated changes of chemical and physical composition. This computer code (Stathopoulou and Assimakopoulos, 2005) has been used in Greece for predicting indoor environment to Athletic Halls with HVAC Ventilation, and IAQ in a dentistry clinic (Helmis *et al*, 2007).

The computer code, calculates the 3-D (three-dimensional) flow field, energy and pollutant concentrations using the continuity, momentum, energy and pollutant transport equations. The equations of the model used were the cartesian, partial differential equations (PDEs) for the conservation of mass, linear momentum, energy and other fluid-dynamics variables in a steady state and turbulent flow (Launder and Spalding, 1972; Launder and Spalding, 1974; Spalding, 1980; Markatos, 1987; Panagopoulos and Markatos, 1991). The independent variables of the problem were the three components x, y and z of a Cartesian frame of reference. The dependent variables were the three components of the velocity vector (v), pressure, temperature and concentration of indoor air pollutants contaminants. Under steady-state conditions, the conservation equations for the mean value of every dependent variable, Φ, can be expressed in the following differential general form:

$$\mathrm{div}(\rho v\Phi - \Gamma_{\mathrm{eff}}\,\mathrm{grad}\Phi) = S_{\Phi} \quad (1)$$

where ρ is the density, Γ_{eff} is the "effective" exchange coefficient of variable Φ and S_{Φ} is the source term for Φ per unit volume. PDEs (1) were integrated over control volumes yielding a set of algebraic equations, the finite-domain equations (FDEs). FDEs were solved using the SIMPLEST algorithm (Patankar and Spalding, 1972). The difference of this algorithm from the well-known SIMPLE algorithm is that the coefficients of the FDEs for the momentum equations contain only the diffusion terms, while the convection terms are added to the linearized sources of the equations. More details of the solution algorithm can be found in the literature (Patankar and Spalding, 1972; Launder and Spalding, 1974; CHAM, 2002).

Turbulence Model Details

It was assumed that indoor flow was buoyant and turbulent because of the kitchen heating source. The well known κ-ε turbulence model with buoyancy terms for κ-ε (Markatos *et al*, 1982; Markatos, 1987; CHAM, 2002) was used.

Boundary Conditions

Input Parameters

Calculations have been performed for various inlet velocities and positions (Scenario A inlet at window, Scenario B inlet at hole 1 and Scenario C inlet at hole 2 as presented in Fig. 2), which corresponded to various indoor velocity vector distributions. Uniform velocities were applied at the inlets, while inlet temperature is set at 20°C, level of the kinetic energy of turbulence κ was set at 0.25% of the mean flow, and the turbulence energy dissipation rate ε was estimated assuming that turbulent viscosity was 1000 times the laminar one. Inlet concentrations of pollutants were set to 305 ppm/600 $\mu g/m^3$, 40 $\mu g/m^3$, 50 $\mu g/m^3$, 5 $\mu g/m^3$ for CO_2, NO_2, VOC and formaldehyde respectively. Inlet Boundary conditions (BC) parameters set for flow, temperature and contaminants are presented in the following Table 1.

Overall Ventilation Rate and Reference Temperature

The set up of inlet BC for uniform velocities for all cases corresponded to overall ventilation rate of 324 m^3/h, 3.3 m^3/m^2h and 9.9 ACH (air changes per hour) in compliance with California/USA regulations (for minimum design ventilation California Title 24 suggests 3 m^3/m^2h based on ventilation surface for the whole apartment) and ASHRAE Standards (for local ventilation ASHRAE Standard 62.2-2003 suggests kitchen exhaust airflow rates 5 ACH based on kitchen volume).

It was assumed that indoor airflow was turbulent with buoyancy force because of the kitchen heating source. For the buoyancy term a reference temperature based on the inlet temperature 20°C was set.

Boundary Conditions for the Cooker and Reference Hood

The source of energy due to the cooker activities was set at 1500 W (1.5 kW) while relevant pollutants emissions due to the cooker activities were set to 0.34 kg/h, 50 mg NO_2/kWh, 50 mg VOC/kWh for CO_2, NO_2, and VOC respectively according to guidelines published by Environment Australia (Environment Australia, 2001).

Boundary Conditions for Floor Surfaces

The floor pollutants emissions for VOCs and formaldehyde were set to 0.28 $\mu g/m^2s$ and 0.08 $\mu g/m^2s$ respectively according to guidelines published by Environment Australia (Environment Australia, 2001).

Boundary Conditions for Walls

For the wall surfaces the no-slip condition was applied for velocities and "wall functions" for the near-wall values of the dependent variables κ, ε and temperature. Zero gradient BC were set for pollutants concentrations variables. Walls were assumed not to emit VOCs and formaldehyde, based on the assumption that water-based paints were used.

Output Parameters

As pointed out calculations have been performed for various magnitudes of inlet velocities and inlet positions (Scenario A inlet at window, Scenario B inlet at hole 1 and Scenario C inlet at hole 2 as presented in Fig. 2), which corresponded to various indoor velocity vector distributions. A zero reference external pressure was applied as output BC.

Table 1. Inlet Boundary Conditions for flow, energy and contaminants.

Scenario	AIR VELOCITY (m/s)			TEMPERATURE (°C)	POLLUTANTS ($\mu g/m^3$)			
	WINDOW	HOLE1	HOLE2		CO_2	NO_2	VOC	Formal
A	0.15			20°C	600	40	50	5
B		2		20°C	600	40	50	5
C			2	20°C	600	40	50	5

COMPUTATIONAL DOMAIN AND COMPUTATIONAL DETAILS

The simulation model geometry has been constructed using CAD files. A rather coarse grid was used in the computations, which covered a computational domain measured 4.96 × 9.78 × 3.00 m. The non-uniform numerical grid consisted of 171990 differential volumes, 63 cells in the x direction, 65 cells in the y direction and 42 cells in the z direction. The grid covered that part of the apartment which consists of the kitchen and the living room with the provision of obstacles present.

Almost 3000 iterative sweeps of the domain were necessary to obtain convergence. The computer used was an AMD Athlon 64 Processor 3200 + 2.0 GHz. Memory RAM used was 512 MB. Execution times per 1000 sweeps for the calculation grid were around 1 hours CPU. The grid was optimum in terms of computational efficiency versus CPU time, between three sets of increasing complexity.

RESULTS AND DISCUSSION

Results

Results for the flow field and the indoor pollutants concentrations for scenarios A, B and C are presented in Figs. 3 to 6 (along the plane A-A' depicted in Fig. 1) and major results are presented in tabulated manner in Table 2.

Observation of the above figures results to the following conclusions:

- The predicted velocities and contaminants fields are physically realistic and plausible.
- Scenario A performs better while scenarios B and C perform poorer due to the creation of vortices related to jet inflows from the holes. Inlet air location is critical since local recirculation and "hot-spots" of stagnant air can appear within the apartment.

Discussion-Conclusions

The methodology that was applied provides qualitative and quantitative data in order to evaluate and select measures and techniques that ensure the prevention of adverse indoor environmental impacts and the protection of human health. The mathematical model analysis employed provides the basis in achieving ***best practice environmental management*** in order to implement relevant indoor air pollution projects. It can also assist decision-making and provides greater certainty to the construction firms and the community in carrying out planning for Indoor Air Pollution activities, by examining the detailed behavior of alternative design in a short time and with minor cost.

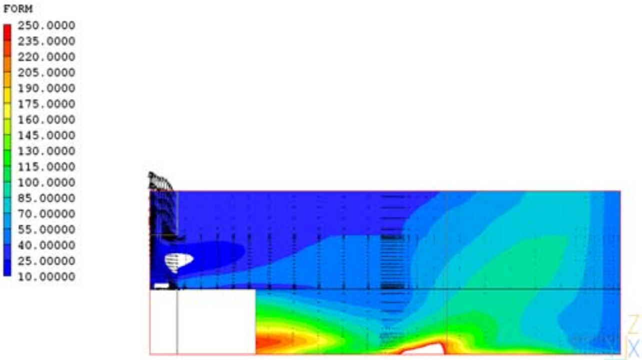

Fig. 3. Concentration of Formaldehyde at y-z plane, CASE A [x = 2.18 m, unit; μg/m^3] with velocity vectors.

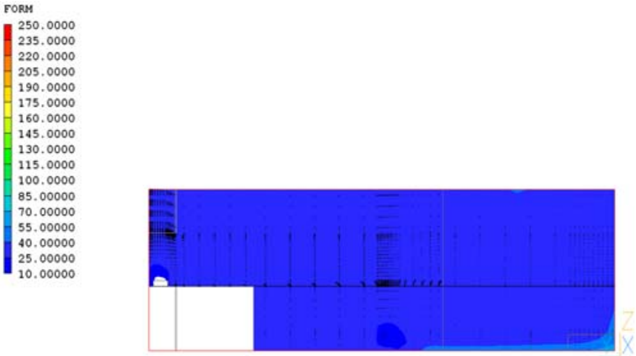

Fig. 4. Concentration of Formaldehyde at y-z plane, CASE B [x = 2.18m, unit; μg/m^3] with velocity vectors.

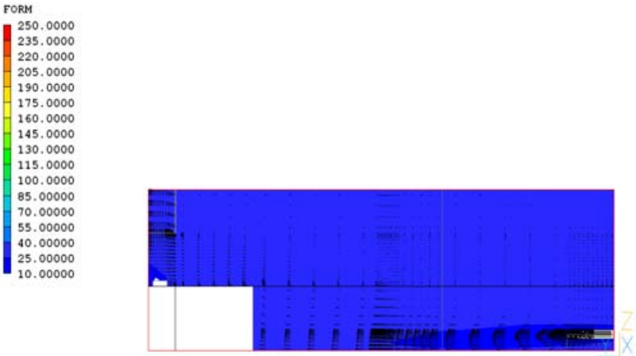

Fig. 5. Concentration of Formaldehyde at y-z plane, CASE C [x = 2.18 m, unit; μg/m^3] with velocity vectors

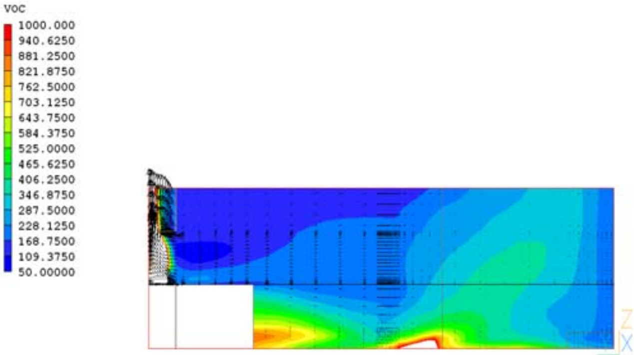

Fig. 6. Concentration of VOC at y-z plane, CASE A [x = 2.18 m, unit; μg/m^3] with velocity vectors

The method proposed consists a state-of-the-art tool in the direction of employing CFD methodology to improve indoor pollution and ventilation techniques, namely focusing on the optimum sizing and siting of ventilation schemes and provision of practical suggestions as a part of an Indoor Pollution Management System.

Table 2. Computational Fluid Dynamics model major results.

Scenario	Computation Fluid Dynamics model major results for pollutants VOC and Formaldehyde.
A	Total pollutant discharge through hood – Pollutant is not convected into the main kitchen room volume.
B	Although the main pollutant discharge is achieved through the hood, some pollutant escapes and is convected into the main kitchen room volume (About the half of it) and flows by a vortex (at the x-z plane) created by the inlet-hole 1 opening inflow.
C	Although the main pollutant discharge is achieved through the hood, some pollutant escapes and is convected into the main kitchen room volume (most of it) and flows by a vortex (at the y-z plane) created by the inlet-hole 2 opening inflow.

REFERENCES

American Society of Heating Refrigerating and Air Conditioning Engineers (ASHRAE). (2003). ANSI/ ASHRAE Standard 62.2-2003: Ventilation and Acceptable Indoor Air Quality in Low-Rise Residential Buildings, Atlanta, GA, ASHRAE.

Center for Building Science News CBS (1995). VOCs Exposure Metrics and Sick Building Syndrome. *CBS Newsletter.* 6: 6–9.

CHAM (2002). *Phoenics-VR 3.5 Reference Guide*, CHAM ltd, London, UK.

De Bellie, L., Haghighat, F. and Zhang, Y. (1995). *Review of the Effect of Environmental Parameters on Material Emissions,* Proceedings of the 2nd International Conference on Indoor Air Quality, Ventilation, and Energy Conservation in Buildings, Montreal, p. 111–119.

Environment Australia (2001). *Air Toxics and Indoor Air Quality in Australia,* State of Knowledge Report, ISBN 0 6425 4739.

Godish, T. (1988). Residential Formaldehyde Contamination: Sources and Levels. *Comments Toxicol.* 2: 115–134.

Helmis, C.G., Tzoutzas, J., Flocas, H.A., Panis, V., Stathopoulou, O.I., Assimakopoulos, V.D., Halios, C.H., Apostolatou, M., Sgouros, G. and Adam, E. (2007). Indoor Air Quality in a Dentistry Clinic. *Sci. Total Environ.* 377: 349–365.

Launder, B.E. and Spalding, D.B. (1972). *Mathematical Models of Turbulence,* Academic Press, London.

Launder, B.E. and Spalding, D.B. (1974). The Numerical Computation of Turbulent Flows. *Comput. Meth. Appl. Mech. Eng.* 3: 269–289.

Markatos, N.C. (1987). Computer Simulation Techniques for Turbulent Flows, In *Encyclopedia of Fluid Mechanics. Vol. 6: Complex Flow Phenomena and Modeling*, GULF Publishing Company, Houston.

Markatos, N.C., Rhodes, N. and Tachell, D.G. (1982). *Numerical Methods for Fluid Dynamics,* Morton, K.W. and Baines, M.J. (Eds.), Academic Press, London.

Panagopoulos, G. and. Markatos, N.C. (1981). *A Method of Assessing the Contribution of Various Pollution Sources through Mathematical Modelling*, International Conference on Environmental Pollution, Lisbon.

Patankar, S.V. and Spalding D.B. (1972). A Calculation Procedure for Heat, Mass and Momentum Transfer in Three-Dimensional Parabolic Flows. *Int. J. Heat Mass Transfer* 21: 1787–1806.

See, S.W, and Balasubramanian, R. (2006). Physical Characteristics of Ultrafine Particles Emitted from Different Gas Cooking Methods. *Aerosol Air Qual. Res.* 6: 82–92.

Spalding, D.B. (1980). *Mathematical Modeling of Fluid Mechanics, Heat Transfer and Mass Transfer Processes.* Report HTS/80/1. Imperial College CFDU.

Stathopoulou, O.I. and Assimakopoulos, V.D. (2005). Application of PHOENICS to Athletic Halls with HVAC Ventilation, Proc. Int. Conf. Ventilation in Relation to the Energy Performance of Buildings, IEA and AIVC (Eds.), Brussels, Belgium.

United States Environmental Protection Agency. Office of Air and Radiation (OAR). Indoor Environments Division. (1997). An Office Building Occupant's Guide to Indoor Air Quality. EPA-402-K-97-003.

United States Environmental Protection Agency. Office of Air and Radiation (OAR). Indoor Environments Division. (1995). Characterizing Air Emissions from Indoor Sources. EPA-600-F-95-005.

United States Environmental Protection Agency. Research and Development. (1991). Indoor Air Facts. Sick Building Syndrome. *MD-56.*

United States State of California Legislation. (2001). California Title 24 Standards, CCR, Title 24, Part 6, Sec. 121(b) 2.

Wang, H.K., Huang, C.H., Chen, K.S. and Peng, V.P. (2010). Seasonal Variation and Source Apportionment of Atmospheric Carbonyl Compounds in Urban Kaohsiung. Taiwan. *Aerosol Air Qual. Res.* 10: 559–570.

Received for review, November 1, 2010
Accepted, January 25, 2011