



CHAM Limited

Summer 2010

PHOENICS News

Professor Spalding Receives Franklin Medal

The week of April 22 was Franklin Awards Week in Philadelphia. The Franklin Institute's mission is to inspire "a passion for learning about science and technology". To this end it presents annual awards to those who have achieved excellence in various scientific fields (www.fi.edu).

Professor Spalding's award, in Mechanical Engineering, was for his "seminal contributions to the computer modelling of fluid flow, creating the practice of computational fluid dynamics (CFD) in industry, and paving the path for the widespread application of CFD to the design of objects from airplanes to heart valves."

During the week, Professor Spalding spent time at the Franklin Institute with a display of PHOENICS applications which could be viewed by young visitors to the Museum who were encouraged to ask questions. He also delivered a lecture on *Benjamin Franklin & CFD* (www.cham.co.uk/lectures) as part of a CFD-related program at Villanova University arranged by his sponsor, Dr Gerard Jones. Four past students attended: Steven Beale & Andrew Pollard drove down from Canada, Akshai Runchal came from California (via India), Malcolm Andrews flew in from Texas.

On presentation day a formal reception was followed by the ceremony featuring a video concerning the lives and achievements of each Laureate (www.cham.co.uk/news).

Laureates received their medal from the President of the Franklin Institute, Dennis Wint. After the ceremony Bill Gates, the 2010 winner for Business Leadership, spoke briefly. Laureates then processed out and were joined by some 800 guests for a formal banquet – a truly memorable occasion.



Professor Spalding & Sponsor Dr Gerard Jones



Franklin Medal Certificate



The Franklin Institute



Brian Spalding & Dr Gerard Jones



Villanova Lecturers



Steven Beale, Andrew Pollard, Professor Spalding, Akshai Runchal & Malcolm Andrews



Drs Jones & Runchal: Technical Discussions after dinner

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Special points of interest:

- **The Franklin Award**
- **PHOENICS Modelling of Data Centres at CHAM**
- **PHOENICS Used to Model Upper Respiratory Tracts in Japan**
- **PHOENICS Used to Model Air Pollution in Tunnels**

2. PHOENICS Applications

2.1 Implementation of a Collision Model between Magnetic and Neutral Particles in PHOENICS by Hiroji Suzuki, ITOCHU Corporation, Tokyo, Japan

1. Introduction

The collision model between magnetic and neutral particles is implemented in PHOENICS 3.5.1 by using the users subroutine (Ground) to simulate the phenomenon of extracting the neutral particle. The confirmation calculation is done, considering the free surface (SURF), by a 2D cylindrical model (Fig.1). The Lagrangian method is used to compute movement of the particles. The lower part of the cylindrical receptacle is filled with water. The magnetic particles and the neutral particles are made a clear distinction in the low part for the initial condition.

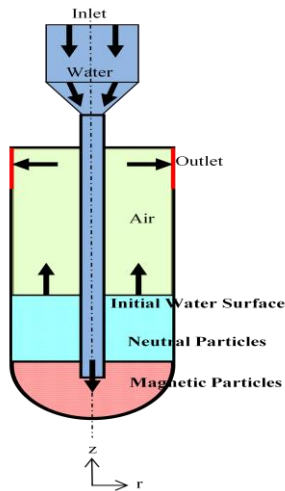


Fig.1 Computational Model

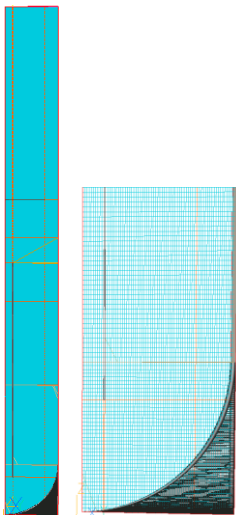


Fig.2 2D Cylindrical Mesh

2. Particle Model

The following particle model is implemented in PHOENICS 3.5.1

- Three kinds of particles are considered (magnetic, neutral and neutral including magnetic via the collision).
- Particle movement is computed by Newton's equation of motion.
- Drag force between particle and fluid is considered for the particle only.
- The magnetic force operated for the magnetic particle depends on the position(r, z) of the particle.
- The buoyancy force is considered for the particle.
- KIVA[1] is used for the collision model.
- The collision between particle and wall is elastic.
- Brownian motion of a particle is considered.

3. Coordinate System of a Particle

A normal coordinate system is used to compute the equation of motion for the particle. The position of the particle in the normal coordinate system is computed from the position in the physical coordinate system by the mapping transformation used for any coordinate systems (Cartesian, Cylindrical, BFC).

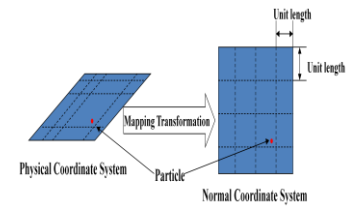


Fig.3 Mapping Transformation

4 Computational Conditions

4.1 Computational Conditions for Fluid

The computational condition for fluid is given below.

- Coordinate system is a 2D cylindrical system (Fig.2)
- Computational meshes are: 15,975($NX \times NY \times NZ = 1 \times 71 \times 225$)
- Unit system is (mm,mg,sec)
- Time step size for fluid is 1.0E-4[sec] (3,000[step] for 0.3[sec])

- Time step size for particle is 1.0E-5[sec]
- Property of fluid
 - Density: 9.9823E-01 [mg/mm³] (Water)
 - 1.189E-03 [mg/mm³] (Air)
 - Kinematic viscosity: 1[mm²/s] (Water)
 - 1.544E+01[mm²/s] (Air)
- Boundary condition
 - Inlet : Inlet velocity 5[mm/s]
 - Outlet : gauge pressure 0[mm/(mm*s²)]
 - Wall : Non-slip

4.2 Computational Conditions for Particles

The particle computational condition is given below:

- Initial condition
 - Magnetic particle: 10,000 computational particles in red region (Fig.1).

A computational particle expresses 673 real particles. Neutral particles: 10,000 computational particles in blue region (Fig.1).

A computational particle expresses 12 real particles.

Magnetic and neutral particles are placed uniformly by using random numbers for the location for each particle.

- Particle Radius: Magnetic: 0.1[μm]; Neutral: 10[μm]
- Particle Density: Magnetic: 7.87[mg/mm³]; Neutral: 0.99823[mg/mm³]
- Gravitational acceleration: g: 9810[mm/sec²] for -z direction

4.3. Results

Particle distribution is shown in Fig.4-Fig.7. Red indicates magnetic particles, black indicates neutral particles and green indicates neutral including magnetic from the collision.

The neutral (green) particles are distributed between magnetic and neutral particles, because they are created by the collision.

Picture files for Figs.4-7 are created using the PHOTON GEOMETRY feature. The shape of the particle is a very small triangle.

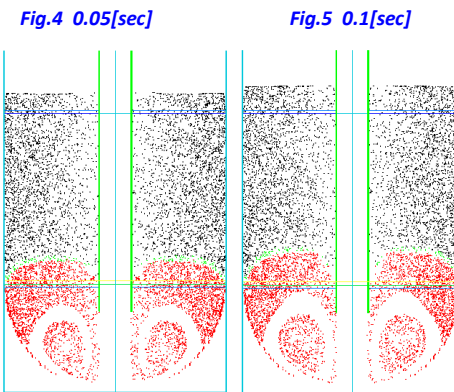
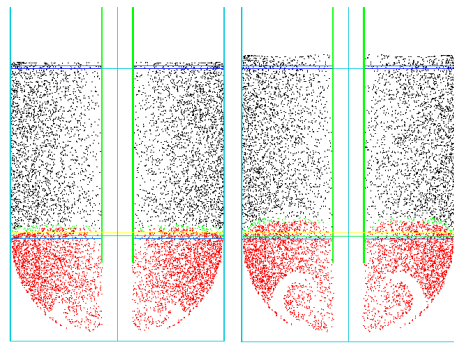


Figure 8 shows distribution of the fluid velocity vector.

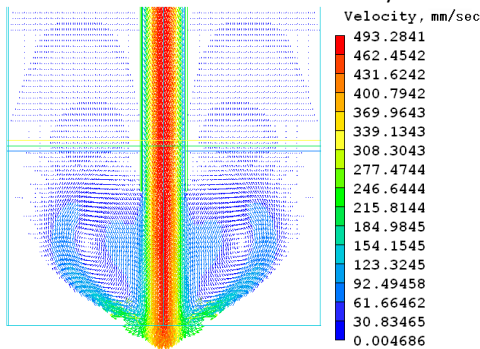


Fig.8 Velocity Vector of Liquid at the bottom part (0.2[sec])

5. Conclusions

The following problem remains now.

- The collision frequency has not yet been confirmed by comparing this result with the experimental data.
- When this 2D cylindrical model with free surface (SURF) is used, it takes nearly 10 days to compute a phenomenon which takes a few seconds to occur.

The above problems will be resolved as follows

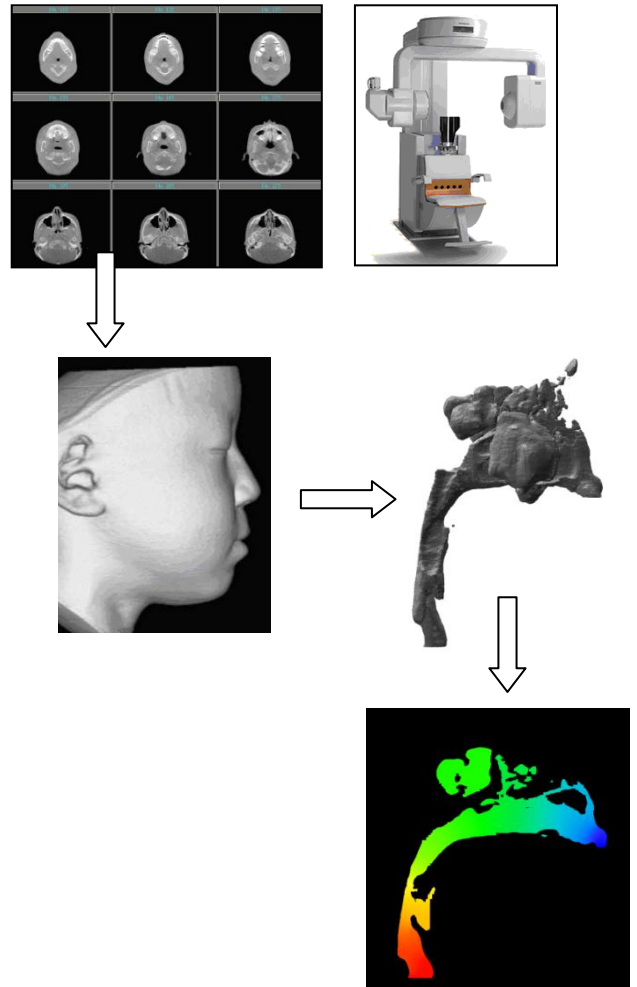
- It is possible to confirm the collision model by getting the experimental data.
- It is possible to shorten computational time for free surface by using simple free surface model (Moving Porosity or HOL)

6. References

- 1] A. A. Amsden, J. D. Ramshaw, P. J. O'Rourke, and J. K. Dukowicz, KIVA: A Computer Program for Two- and Three-Dimensional Fluid Flows with Chemical Reactions and Fuel Sprays, Los Alamos Indentification No. LP-1462.
- 2] Kanji Takahashi, Basic Aerosol Engineering, by Yohkendo Shoten, 1982, pp. 29-32

2.2 Simulation of Turbulent flow to Estimate Virtual Airflow Patterns in the Upper Airway by Tomonori Iwasaka of Kagoshima University Graduate School, Medical & Dental Sciences submitted by Zuwei Kong of CHAM Japan

This research simulates turbulent flow to estimate virtual airflow patterns in the upper airway. Volume rendering software (INTAGE Volume Editor, KGT, Tokyo, Japan) was used to create the 3-D images of the shape of upper airway. The rendered volume data was in a 512×512 matrix with a voxel size of 0.377 mm. The 3-D CBCT images for the airway model were exported to computational fluid-dynamic software (PHOENICS, CHAM-Japan , Tokyo, Japan) in stereolithographic format.

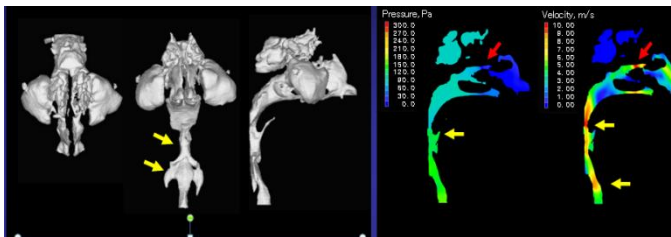
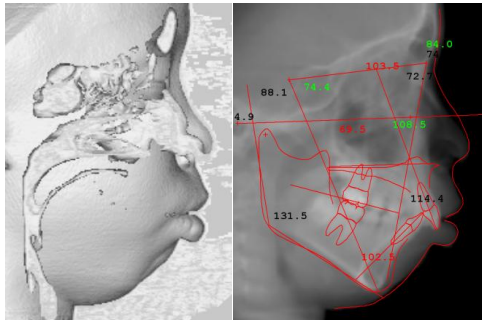


Airway resistance is greater during expiration than inspiration during quiet breathing. Accordingly, each voxel on the plane of the hypopharynx was considered part of the flow inlet while each voxel at the entrance of each nostril was considered part of the flow outlet. The air was assumed to be a Newtonian, homogeneous, and incompressible fluid. Elliptic-staggered equations and the continuity equation were used in the study. The following boundary conditions were set to the model:

- 1) The air flowed perpendicular to the lower pharyngeal plane had a velocity of 200 ml/sec.
- 2) The wall surface was non-slip.
- 3) The simulation was repeated 1000 times to calculate the mean values. Convergence was judged by monitoring the magnitude of the absolute residual sources of mass and momentum, normalized by the respective inlet fluxes.

The iteration was continued until all residuals fell below 0.2 %.The results of the FMS are shown as pressure and velocity. The maximum pressure and the maximum velocity of the upper airway were calculated to evaluate the ventilatory condition and to detect obstructions in the upper airway.

Case result picture:



Reference:

- 1) Iwasaki T, Hayasaki H, Kanomi R, Saitoh I, Yamasaki Y: Dental influences of upper airway obstruction on facial skeletal morphology in children with use of fluid-mechanical simulation. Pediatric Otorhinolaryngology Japan. 2009. 30(1): 5-9.

3) Consultancy Applications

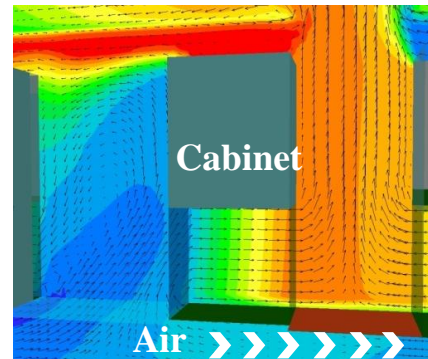
3.1 Modelling of Data Centres to Optimise Design by Paul Emerson of CHAM Limited

CHAM's consultancy team has been busy working on a variety of interesting projects over the last few months. Much of this time has been devoted to the modelling of data centres to assist with and optimise the design of cooling and ventilation systems, and look at the impact of additional IT loading or investigate cooling failure scenarios.

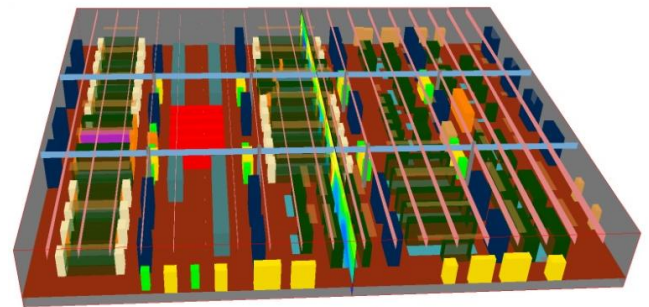


Data centres located across the globe have been simulated, involving complex single or multi room layouts, under-floor ventilation, sometimes a return air ceiling plenum and cold aisle containment systems. CHAM personnel and agents have performed site surveys, gathering detailed information on the layouts and cooling systems, which, together with engineering drawings, enabled 3-D models to be built using CHAM's streamlined method.

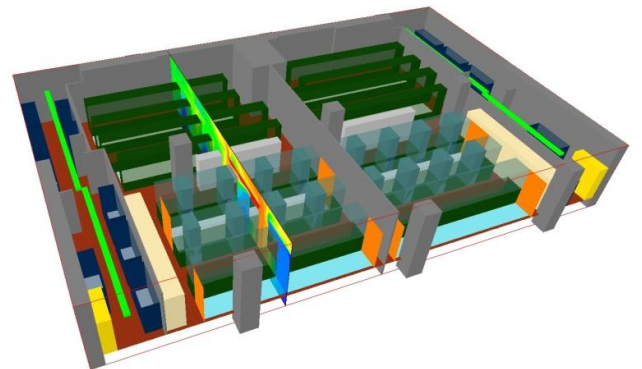
This method constructs a list of the data centre contents together with key parameters (e.g. air flow rates, heat output) within a single spreadsheet. The spreadsheet is read by PHOENICS, enabling common data centre objects (i.e. CRACs, PDUs, cabinets, floor/ceiling grilles) to be constructed automatically. It allows rapid changes to be affected, such as scaling IT loads by changing a single value in the spreadsheet.



Results from the simulations show the air flows and temperatures into and out of the cabinets, indicating undesirable regions of recirculation from hot to cold aisles. PHOENICS also enables average and maximum inlet and outlet temperatures to all cabinets to be evaluated.



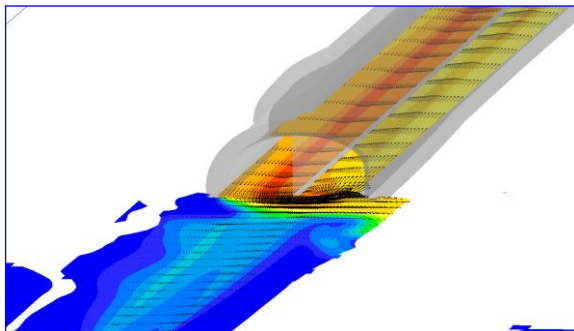
The predicted power output from any chilling device can be determined and is useful for highlighting which units are not providing sufficient cooling, and which are only partially loaded. Results might indicate a re-distribution of the units to optimise the cooling, or even fewer units required thus providing cost savings.



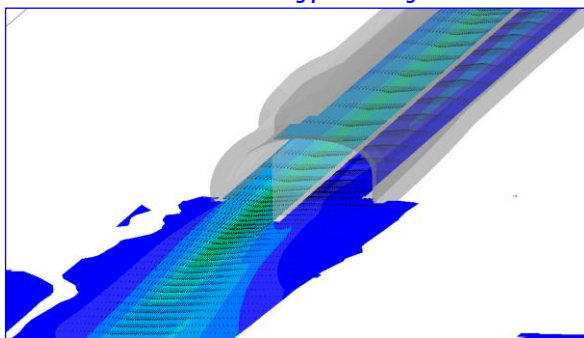
Initially the required air flow rate through each floor or ceiling grille is estimated, but often the results from the CFD simulation will show some re-balancing is necessary to achieve good air distribution throughout the room. This re-balancing can be achieved using CFD, and is useful during the commissioning process when the grille flow dampers have to be set. Many of the data centres modelled are to be tested during commissioning, with measurements taken which will provide useful data to help validate the CFD results.

Cooling systems are resilient, so in the event of one or more units failing there is sufficient capacity available to continue operation at full load. Simulations during failure scenarios have been undertaken to investigate the air distribution across a data centre when one or more chilling units fail. In addition, there are plans to simulate conditions during a power outage, when IT loads are maintained throughout the outage (by Uninterrupted Power Supply systems), but the cooling system drops off for a short time whilst the backup generators come on-line. Transient or time-dependent CFD calculations would allow the environment within all cabinets to be monitored during this outage.

3.2 Road Tunnel NO_x Reduction by Kate Taylor of CHAM Limited



NO₂ concentration - existing portal design



NO₂ concentration - extended partition

Air pollution from vehicle exhausts is a serious public health issue, particularly in road tunnels where pollutants may be concentrated at harmful levels. Long tunnels may require significant forced ventilation to keep pollution below maximum safe levels, with tunnel portal geometry and surrounding topography also affecting the dispersion of pollutants.

CHAM recently undertook a consultancy project on behalf of CFD Service AB in Sweden to investigate the ventilation of a 1.2 km road tunnel near Stockholm. The tunnel was a single bore design with a central partition to separate two lanes of opposing traffic flow. Despite using ventilation fans to draw air through each lane of the tunnel NO₂ concentrations were found to be higher than expected due to reingestion of the exhaust flow from one lane back into the tunnel in the opposite lane.

A PHOENICS model of the tunnel was constructed using CAD of the tunnel geometry and topography surrounding the portals. The model included ventilation fans within the tunnel and sources to represent vehicle drag and NO₂ production. Local wind conditions around the tunnel site were also included in the model.

The model was initially run using the existing tunnel and portal geometry to ascertain that the CFD could reproduce measured air velocity and NO₂ concentrations. The CFD quite clearly showed the re-ingestion at both ends of the tunnel, and how little fresh air from the surroundings was drawn into the tunnel mouth - consequently the NO₂ concentration built up within the tunnel. Various modifications were then made to the model to try to restrict this re-ingestion - the most obviously successful being an extension of the central partition separating the two lanes of traffic beyond the tunnel mouth at each end. In this case the NO₂ level still increased along the tunnel, but the overall level was much lower because clean air is entrained at each entrance. The CFD model was then used to optimise the length and height of partition required.

4) Technical News & User Applications from Agents

4.1 Coolplug and the German Market: A Retrospective View of 2009 and the Outlook for 2010 by Frank Kanter

Despite the financial crisis, 2009 has been a good business year for Coolplug and PHOENICS in Germany. Revenue for the calendar year increased by 70% due to a number of new customers. Almost all of these new customers are planning offices in the field of the building services engineering industry. PHOENICS/FLAIR is market leader in this area in Germany and this industry is booming due to the following reasons.

1) Modern Architecture

Atria and glass facades, for example, make it difficult to get the right comfort due to solar radiation and complicated air flows. Conventional tools, like TAS from EDSL, are not sufficient anymore and CFD is needed in the planning phase. A nice example of this is "BMW Welt" in Munich where PHOENICS has been used for various calculations (e.g. dispersal of pollutants, wind loads).



Picture 1: BMW Welt, Munich

2) Wind simulations

Calculation methods for wind loads on buildings are based on simple geometries. In Germany the DIN 1055-4 03/2005 (German industry norm) is used for this. However, for buildings with a more complicated shape, so almost every new tower, this cannot be applied anymore. Wind channel measurements or CFD calculations need to be performed. In Hamburg the local authority approved PHOENICS, after a validation study, to be used for wind loads calculations for the Central Plaza Tower.



Picture 2: Central Plaza Tower, Hamburg

3) Investments in the Middle and Far East especially China

German planning offices have a very good reputation in the world. In the booming industries of the Middle and Far East a lot of modern, big buildings are planned to be build, where German companies are involved in the design of the HVAC systems. A great opportunity for PHOENICS!

For 2010 my expectation is that the growth in the building service engineering market will compensate for the cost savings that many companies are planning to make. Some companies will probably put software maintenance on hold; others are looking to open source alternatives. A main goal of Coolplug will be to convince current customers that these kinds of savings will not help reduce costs and eventually will increase them. A better strategy will be to try to increase the amount of work for PHOENICS. Coolplug will help them by organizing the following:

1. new website with a lot of tips and tricks targeted to the German market.
2. user day in September/October this year, details to follow.



Frank Kanthers, Coolplug BV

3. free publicity by supplying journalists with PHOENICS examples for their publications in order to establish PHOENICS reputation. A recent example is an article in Deutsches IngenieurBlatt about wind load calculations.

4.2 The French Market: Contributions from French Users submitted by Jalil Ouazzani

1) Impact of a tyre fire on an LPG tank by Dr. André Carrau, FASIS

The accident analysis shows that different truck-tyre fires have occurred in recent years, some resulting in the death of the driver due to a tyre explosion. In the case of a tank containing LPG, it also raises the question of the risk of BLEVE during a tyre fire.

In this context, FASIS (Industrial Safety Facilitators) conducted an experimental and numerical project to study the impact of a tyre fire on a tank containing LPG.

Phase 1: Full-scale experiment.

The test was conducted in a test hall. It focused on the burning of a tyre on an LPG tank with a capacity of approximately 51 m^3 . The tank contained only air for safety reasons.

The temperature of the tank wall (inside and outside), the temperature inside the tank and in the environment were measured (forty measurement points). The central tyre was first ignited (with 1 litre of heptane).

The experiment revealed two distinct phases. During the first phase, the fire spread from the central tyre to the rear tyre and then began to diminish until the violent explosion of the central tyre (after 25 minutes). Then, the fire began to spread again until the explosion of the second tyre (50 minutes).

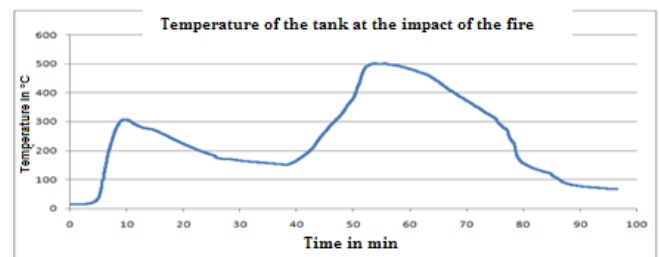


Fire after 10 minutes



Second explosion

The following curve shows the temperature of the tank, measured at the impact point of the fire above the central tyre.



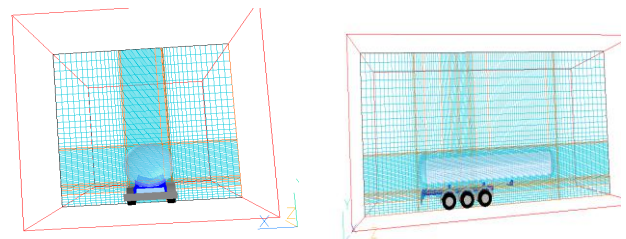
Phase 2 : Numerical approach

The first step was to calibrate PHOENICS software with the experiment.

The non stationary Navier-Stokes equations with the Chen and Kim turbulence model were employed.

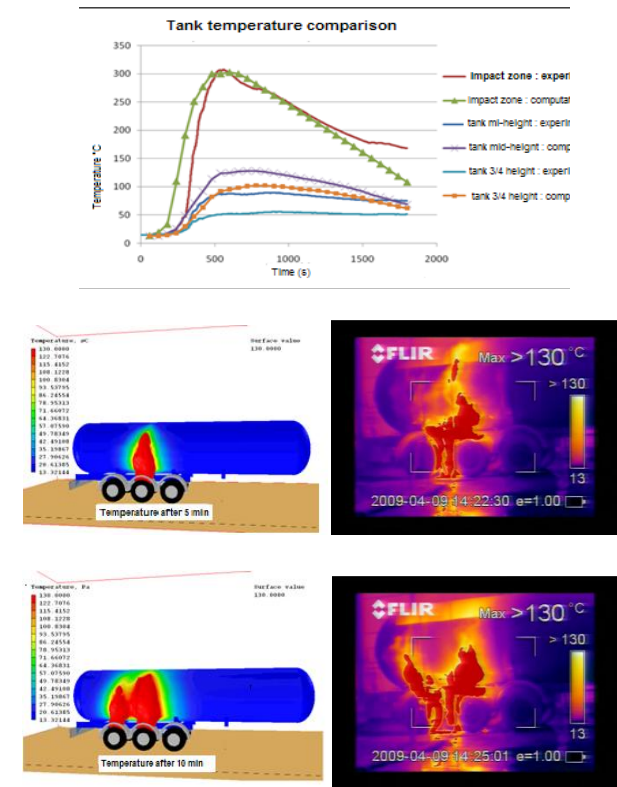
The computation of the conduction through the thickness of the steel presented some difficulties due to its thickness. To remedy the situation, the thickness of the tank was artificially increased by a factor of 10. The steel properties (conductivity, specific heat, density) were modified to reproduce the same heat transfer.

The mesh used was a structured mesh with more than 600 000 cells.



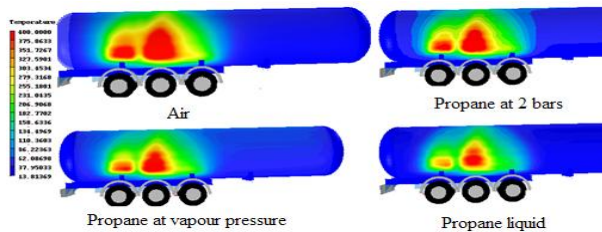
Comparison was made on the first half-hour of the experiment. In the computation, the fire was represented by a volume source term. The heat release rate of the tyre was deduced from measurements of heat fluxes.

The following figure represents a comparison of the wall temperature above the central tyre. The computation result is in good accordance with the experimental results.



Comparison at 5 min and 10 min : computation and experiment (infrared camera)

After comparison, we studied the influence of the contents of the tank to the temperature levels. For this we considered the case of a tank full of propane or butane gas at different pressure levels, full of liquid propane and gas (82% liquid) and full of butane liquid gas (82% liquid). In the case of a tank containing liquid and gas it wasn't considered a two-phase model. The gas and liquid phases were treated as independent phases. The following picture represents a comparison of the temperature wall depending on the tank contents.



Conclusion

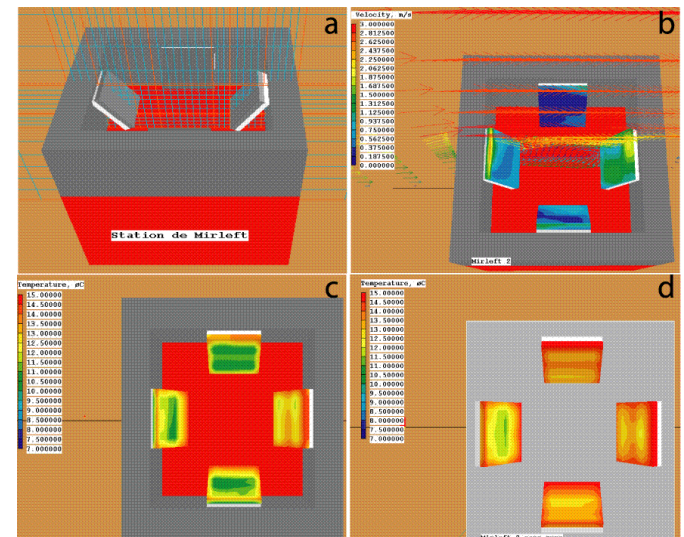
To study the impact of a tyre fire on a tank, a double approach experience-computation was conducted. The comparison with the full-scale showed the ability of PHOENICS to model this type of phenomenon. Following the comparison with the experiment, the influence of the tank contents on the temperature levels was explored with PHOENICS. However, the model needs to be improved to take into account the phenomena of liquefaction or vaporization inside the tank.

A special thanks to Dr J. Ouazzani of Arcofluid for his support in the definition and setting up of the problem in the PHOENICS code.

2) Radiation-Cooled Dew Condensers in the South of Morocco Using CFD by Imad LeKouch, University of Agadir Morocco & ESPCI (Paris) and Jalil Ouazzani, Arcofluid, France

Radiation-cooled dew water condensers can serve as a complementary potable water source. In order to enhance passive dew collection water yield, the Computational Fluid Dynamics (CFD) software, PHOENICS, was used to simulate several innovative condenser structures in the area of Mirleft (South of Morocco). The sky radiation is calculated for each of the geometries. Several types of condensers under typical meteorological conditions were investigated using their average radiating surface temperatures.

The simulations were compared with dew yield measurements from a 1 m² 30°-inclined planar condenser used as a reference. A robust correlation between the condenser cooling ability and the corresponding dew yield was found. The following shapes in flat roofs typical of Moroccan houses were studied; four inclined condensers were installed on a square roof. The model of radiation used is IMMERSOL, with a Chen Kim $k-\epsilon$ model of turbulence.



Mesh, velocity and temperature contours on the four condensers

The equations of momentum, continuity and temperature are solved with the finite volume code PHOENICS [11]. The density variation in the body forces, responsible for free convection, is introduced through the Boussinesq approximation [17]. The algorithm solution of the pressure field, which is essential for the determination of the velocity field, is obtained using the SIMPLEST algorithm based on the SIMPLER algorithm coupled with PARSOL. The latter is the PHOENICS feature that allows the flow around and within bodies of arbitrary shape to be computed on Cartesian grids or polar coordinate grid. It avoids the tedious work of creating a curvilinear structured mesh in body fitted coordinates.

The solid bodies (condensers) are digitized into elementary cells (volume V_c) within a 2 cm size mesh. At the interface with the outer space around the solid bodies, a correction of flux (momentum and energy) must be made around the solid facets that make a non-zero angle with the Cartesian frame of reference. The technique used is a triangulation derived from the well-known "cut and cell" technique. At the interface between the solid body and the outer space, the mesh is made variable according to a precision criterion (relative deviation smaller than 0.1 %).

Both 2D and 3D simulations can be performed. Boundary conditions are given for velocity Cartesian components and temperature. We assume a wind profile with a logarithmic variation in the vertical direction and a fixed air temperature at the inlet of the domain. At the surfaces (ground and condensers) conditions for each case studied are applied for either fixed temperature or flux type (radiative cooling).

In quantifying the ability of radiative condensers to cool down below the surrounding air temperature in the presence of wind, CFD can be a very powerful tool to characterize and compare new designs for dew condensers for specific environmental settings. Details of this work can be found in:

- 1) PHD thesis of Imad Lekouch, " Production d'eau potable par condensation passive de l'humidité atmosphérique (rosée)", February 2010, Univeristy of Agadir & ESPCI (Paris)
- 2) Imad Lekouch, Marc Muselli, Belkacem Kabbachi, Jalil Ouazzani, Iryna Melnytchouk-Milimouk, Daniel Beysens. Dew, fog, rain as supplementary sources of water in south-western Morocco. *Energy*, Mars 2010
- 3) Comparison of various radiation-cooled dew condensers using computational fluid dynamics, O. Clus , J. Ouazzani, M. Muselli ,V.S. Nikolayev, G. Sharan, D. Beysens, *Desalination* 249 (2009) 707–712
- 4) O. Clus, M. Muselli, J. Ouazzani, V. Nikolayev, D. Beysens, CFD numerical and experimental study of dew collectors architecture: cone compared to plane, *Proceedings of the 4th Conference on Fog, Fog Collection and Dew* (La Serena, Chile, 23-27 July 2007), p. 315, 2007.

5) News and Events

5.1 CHAM News

- CHAM is collaborating on an EU-funded Eurostars Project in the field of wind energy, in conjunction with WindSim Norway and Iberdrola of Spain.
- Sebastien Comberbach, a third year M.Eng student at the University of Warwick, has joined CHAM for a three-month placement. We hope he enjoys his time with us and gains experience which will contribute to his studies.
- Students are also expected from King's College School, Wimbledon, of which Professor Spalding is an ex-student himself – and an Honorary Fellow.
- Professor Spalding is busy outside as well as within CHAM. He has been appointed to the Awards Panel of the Global Energy Committee for a further 5 year period and has agreed to edit Section 1 of the Heat Exchanger Data Handbook (HEDH) published by Begell House. He lectured on *Benjamin Franklin and CFD* at the Franklin Awards Ceremony in April and on *PPT and PPB fields, facilitating the comparison of experimental and DNS-, LES-, PANS-, PDF- transport or MFM-model representations of turbulence* at the 8th International ERCOFTAC Symposium in Marseille, June 9-11 2010.

This Newsletter is a platform for you to tell us, and others, what you are doing with PHOENICS. Please email your articles for the Autumn Newsletter to Colleen King, cik@cham.co.uk

5.2 Current and forthcoming Meetings and Even.s

Jun 11 2010	Shanghai User Meeting and Shanghai Expo. 
June 23-15 2010	DMS, 21 st Design Engineering & Manufacturing Solutions Expo, Tokyo, Japan
TBA	Training Courses in Beijing, Shanghai, Xi'an and Shenzhen
	CHAMPION Training Course, Taiwan 
Sep 7-9	PHOENICS Training Course at CHAM (UK). For further information, or to book a place, please contact: sales@cham.co.uk
Sep 28	Dutch User Meeting- Aristo Centre , Eindhoven. For further information contact: phoenics@a2te.nl
Oct	German User Meeting. For further information contact: Frank.Kanters@Coolplug.com
Nov 9-11	 PHOENICS Training Course at CHAM (UK). For further information, or to book a place, please contact: sales@cham.co.uk



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