PHOENICS

News

Spring / Summer 2009

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1) Editorial





Professor Brian Spalding, FRS, FREng Becomes a Global Energy International Award Laureate

President Dmitry Medvedev will make Professor Brian Spalding, an international scientist and Managing Director of CHAM Limited Wimbledon, a Global Energy International Laureate on June 5 2009 in St Petersburg during the International Economic Forum being held in that city (www.forumspb.com).

Professor Spalding is honoured for "numerous original conceptions in the processes of heat and mass transfer which have become the basis for practical calculations of the mechanics of fluid flow" according to Valentin Smirnov, Chairman of the Global Energy Awards Committee.

This prestigious Award was introduced in 2002 at the instigation of leading Russian scientists and with the support of major Russian Energy Companies including Gazprom, United Energy Systems and Yukos and is awarded to scientists for outstanding achievements in the field of



energy. It is intended to encourage effective use of energy resources – a global problem – and to promote cooperation amongst international scientists. (<u>http://www.ge-prize.ru</u>).

Professor Spalding, who is a Foreign Member of the Russian Academy of Sciences and who works closely with a research group at the Moscow Power Engineering Institute, has expressed his delight in receiving the Award, particularly because of his long and close connexion with Russian science and scientists. He becomes one of 17 Laureates to receive the Award to date, chosen from more than 1500 nominated in 2009 for the main energy prize.

Brian Spalding is Managing Director of Concentration Heat and Momentum (CHAM) Limited located in Wimbledon Village for over 30 years. He created the PHOENICS computer-software code which uses Computational Fluid Dynamics to model heat transfer, fluid flow and stresses in solids. Until he retired, Professor Spalding was at Imperial College London as Professor of Heat Transfer and Head of the Computational Fluid Dynamics Unit.

2) Latest PHOENICS Features



When Professor Spalding was invited to address a Conference organized by HTRI (Heat Transfer Research Inc) last year it re-awakened his long-standing interest in Shell-and-Tube Heat Exchangers. He worked on Heat Exchangers at Imperial College and contributed to the Heat Exchanger Data Handbook produced by Hemisphere Publishing in 1990.

Conversations with Heat-Exchanger Designers in Vancouver persuaded Professor Spalding that they could be assisted by a SINGLE PURPOSE program making use of the CFD elements of PHOENICS but requiring users to be expert neither in CFD nor PHOENICS; so he designed the single-purpose Gateway – SHELLFLO.

2.1 SHELLFLO: A New Gateway to PHOENICS Brian Spalding

Most shell-and-tube heat exchangers, throughout the world, are designed using computer programs which, to CFD specialists, appear rather primitive. Thus, instead of calculating the true flow pattern within the shell, they make presumptions based on proposals made by T. Tinker in 1958, namely that the pattern can be characterised as consisting of the 4 streams (A, B, C and E) shown in the following diagram.

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Whether or not this presumption suffices for the prediction of heat transfer rates (probably not, as CFD specialist suppose), it is certainly does not provide answers to questions asked by many designers, such as:

- At what locations are the highest cross-flow velocities to be found (where tube supports may be required to prevent vibration and mechanical failure)?
- Where are the velocities likely to be so low that deposits may settle and cause 'fouling'?
- How can the flow pattern be favourably influenced by the proper placing of impingement plates or changing the 'cut percentage' of the baffles?

Answers can now be provided by a new PHOENICS Gateway - SHELLFLO,

The user interface of SHELLFLO is shown here. Its main structure is that of PRELUDE; and it sends its output to be processed by the EARTH Solver and VR-VIEWER modules of PHOENICS.



However its users require no CFD knowledge; and minimal acquaintance with PHOENICS; for the SHELLFLO Gateway presents only the items which its users need: Inlets, outlets, tube bundles, baffles, impingement plates etc.



Results of **PHOENICS** calculations can be presented to inexperienced users graphically by way of macros. Aided by tutorials, new users soon find that they can extract from them the information which interests them, whether pressure distribution and velocity vectors as above or animated streamlines as below.



SHELLFLO is supplied by CHAM as a stand-alone single-purpose predictive tool, designed solely to assist heat-exchanger designers. The cost of a perpetual licence is competitive with any other similar single-purpose software.

2.2 Hot Tin Roofs and other Thin-Inclined Plate Objects Brian Spalding

Until now, the only thin-plate objects which PHOENICS could introduce were those aligned with grid-co-ordinate directions; for Cartesian grids therefore, they had to be horizontal or vertical. Consequently, when it was desired to simulate an inclined plate, so as to represent for example a pitched roof, it was necessary to introduce an object possessing small but finite thickness. This entailed using a fine grid, so that complete cells were contained within every part of the object; and this in turn led to longer computer times than might otherwise have been needed.

InForm allowed PHOENICS to handle sub-grid-size objects for many years; but, in respect of shape, these have been only points or lines, *ie* zero- or one-dimensional. Recently however the Quadrilateral-Plane object has been added, *ie* a two-dimensional sub-grid-size InForm object.

Such objects are defined by way of the co-ordinates of their vertices, which may be given arbitrary positions consistent with being co-planar; and they may act as obstacles to the flow, or as sources of mass, momentum or energy.

The following diagram illustrates the use of two such objects positioned to create a pitched roof. The planes are drawn in white; and the less-regular red coloration represents PHOTON's attempt to display temperature contours for the rather-too-coarse grid chosen to emphasise that sub-grid-size objects can work in coarse grids as well as fine.



In this case the velocity of air normal to the planes has been set to zero, so as totally to obstruct the flow, and the cells which are cut by them have been given the temperature of 100 degrees. However, other conditions can be set.

InForm objects, of which the shapes are described by formulae, are receiving increasing attention at CHAM, because they do not need to be stored as (sometimes large) .dat files, as do facetted (VR-) objects. Thus, the heater spiral in the following diagram was created simply by typing three lines into the Q1 file.



Current developments in the VR Editor are making these and other InForm capabilities easier for users to exploit.

What's New in PHOENICS 2009 will appear soon on the CHAM Website and in the next Newsletter.

2.3 The WIND Object John Ludwig

When dealing with external flow around buildings, the incoming wind often has a logarithmic (or parabolic) velocity profile. For some time, PHOENICS has had the WIND_PROFILE object which imposed exactly such an inlet profile. However, if the wind direction did not exactly line up with the domain, the user had some arithmetic to perform. A new WIND object performs automatically tasks which, previously, had to be performed manually. It decomposes the wind speed into the velocity components at the domain faces and decides which two faces are upstream inflow boundaries, and which two downstream fixed pressure boundaries. It also obviates the need to perform the calculations again to run the model for a different wind direction.

The attribute dialog of the WIND object is shown here. 'Wind speed' is absolute wind velocity relative to North at the reference height. The 'Angle between Y and North' allows the domain to be aligned with internal objects whilst maintaining true physical orientation. The Editor determines which faces are inflows and which outflow with no further input from users.

| External density is: | Donain f | luid | |
|------------------------|-------------|-------|----|
| External Ambient pr | essure 0.0 | 00000 | P |
| relative to | 1.000E+05 | Pa . | |
| Coefficient | 1000.000 | Line | ar |
| Temperature Ambient | 20.0000 | øC | |
| Wind speed | 10.00000 | m/s | |
| Wind direction | 0.00000 | deg | |
| Reference height | 10.00000 | m | |
| angle between Y and No | orth 0.0003 | co de | J |
| Profile Type | Logarithm | ic | |
| Vertical direction | z | | |
| Effective roughness he | eight 2.00 | 0E-4 | |
| Include open sky | No | | |

If the open sky is included, wind velocity components and turbulence quantities at the top of the domain are computed from the velocity-profile equation. Initial values for velocity and turbulence are also set. The following images show a WIND object used to set external flow conditions around a greenhouse and the new CLIPPING_PLANE object allows the roof to be sliced off to see inside:



2.4 Clipping Plane for VR Editor& Viewer Steve Mortimore

Users can now use the fully functional clipping-planeobject available in the VR Editor and Viewer which can be placed anywhere in the model domain rather than using the near plane to replicate a clipping plane in PHOENICS.

| 29 99860 29 12659 26 25458 27 38287 26 51056 25 63855 24 76654 23 89453 23 02251 27 15051 | | | | |
|--|---|----------------------|-------------|-----|
| 21.27849 20.40648 19.53447 18.65246 17.79045 16.91844 16.04643 | K | General (gases) Save | Page | 1 |
| | | × [Linima d] | Formanda at | A A |

In the Viewer it is optional whether to apply the clipping plane to the plot slices (as well as the objects in the domain). In the image above, the clipping plane is located high up, close to the centre front of the domain. The clipping of the results slices has been turned off.

2.5 PHOENICS to ParaView John Ludwig

ParaView is an open-source, multi-platform data analysis and visualization application. ParaView users can build visualizations to analyze data using qualitative and quantitative techniques quickly. Data exploration can be done interactively in 3D or programmatically using ParaView's batch processing capabilities.

ParaView was developed to analyze extremely large datasets using distributed-memory computing resources. It can be run on supercomputers to analyze datasets of terascale as well as on laptops for smaller data. Under the hood, ParaView uses the Visualization Toolkit (VTK) as the data processing and rendering engine and has a user interface written using Qt[®].

PHOENICS 2009 can output files in VTK format, which can be read and visualized by ParaView. To make the Earth solver write VTK files, click 'Options', 'Additional Interfaces', and select 'Additional VTK output'.

| PHOENICS - VR Edito | r | |
|------------------------|---|--|
| File Settings View Run | Options Compile Build Help | |
| | Solver Monitor Options Run Version • Select Private Solver | <u>₩ ∧ • ≡ □</u> |
| | Change Working Directory Phoenics Environment Setting File Format | |
| | Change Font Text File Editor Background Colour Clear Textbox content | |
| | Addional Interfaces | Additional Teoplot Output Additional FieldView Output Additional VTK Output Additional STL single-file Output Additional individual STL Output |

To visualise the geometry in ParaView, also select 'Additional individual STL output'. This will make the Editor write out an STL file for each object which can be picked up by ParaView. The following images show Library Case V146 visualised in ParaView:



All PHOENICS Users are invited to email articles for inclusion on the CHAM website and in the next Newsletter to <u>cik@cham.co.uk</u>. Thank you.

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3) PHOENICS Development

3.1 InForm Sources for Objects John Ludwig

InForm enables PHOENICS users greatly to extend its capabilities without introducing new FORTRAN coding. Users can express requirements via formulae read by the Input Module (Satellite) and transmitted to the Solver (EARTH) for interpretation and performance of implied computations. Many object types have a button labelled 'InForm Commands' on their attributes page leading to a dialog from which a selection of InForm commands can be attached to the current object. The usual InForm command format is: (KEYWORD of VARIABLE at LOCATION is FORMULA with CONDITION)

- KEYWORD defines what the InForm command sets.
- VARIABLE defines which SOLVEd or STOREd variable it is to apply to.
- LOCATION defines where.
- FORMULA defines what.
- CONDITION sets the conditions under which it will happen.

The new dialog allows the keyword and variable to be chosen from lists, formula and condition are input through an editing window and location is always the current object. Sources added this way replace the 'normal' source produced by the object. For example, to replace the 'plug' velocity profile at an INLET object with a linear profile, double-click the inlet object, click Attributes, then InForm Sources. The following dialog appears:

| In-Form Sources for INLET | | <u>?</u> × |
|---------------------------|--------|------------|
| Add InForm | | |
| | Cancel | ОК |

Click 'Add InForm', and a new line of InForm appears.

| In-Form Sources for INLET | | <u>?</u> [X |
|---------------------------|-----------|-------------|
| Keyword Var | Formula | Condition |
| 1 of is | | with Del |
| Add InForm | | |
| | Cancel OK | |

The desired velocity formula is: W1 = 14*(XG/XULAST + YG/YVLAST). In this formula, XG is the distance of the cell centre in X, XULAST is the domain size in X, YG is the distance of the cell centre in Y, and YVLAST is the domain size in Y. The result is to make the inlet velocity linear in both X and Y. Click the empty button under 'Keyword' to see a list of options:

From the list select 'SOURCE'. Click the empty box under 'Var', a list of currently SOLVEd and STOREd variables appears, select W1 from the list and click OK. To introduce the formula for W1 click the empty box under 'Formula'. An editing window appears:

Place the cursor at the top-left of the input window and type:

14*(XG/XULAST + YG/YVLAST)

then click 'File' and 'Save & Exit'. The new formula appears on the button.

When the inlet velocity is replaced, the mass source should also be replaced otherwise there may be inconsistencies in the pressure field. Mass sources are introduced as sources of the pressure variable, P1.

Click 'Add Inform' again to create a second line of InForm. On the second line, select 'Source' for Keyword and P1 for 'Var'iable. The formula for mass flow is density times velocity. Click Formula for P1 and type in the editing window:

| DEN1*14*() | (G/XULAST + YG/YVLAST) | DEN1 is the |
|---------------------|------------------------|-------------|
| name of the density | store. | |

The default source for an object is a total source for the whole object. Mass flow has been specified as density*velocity, which is in kg/m²/s. To tell InForm that the source is 'per unit area', not total, click the empty box under 'Condition' for P1. In the editing window enter AREA then click 'File', 'Save & Exit'.

The default source form for Inform is a fixed flux. which is fine for mass source which has been specified as a mass flux in $kg/m^2/s$. However, for the W1 velocity only velocity was specified, not momentum flux. To instruct InForm to multiply the velocity (W1) source by the mass (P1) source click 'Condition' for W1 and, in the editing window, enter ONLYMS, 'File', 'Save & Exit'. The InForm Sources dialog should look like this:

| In-Form S | ources for UPSTH | | | | | <u>71×</u> |
|-----------|------------------|---------|-------------------------------|------|-----------|------------|
| | Keyword | Var | Formula | | Condition | |
| 1 | SOURCE | f Pl is | den1*14*(xg/xulast+yg/yvlast) | with | area | Del |
| 2 | SOURCE | f W1 is | 14*(xg/xulast+ yg/yvlast) | with | onlyms | Del |
| | | | | | | |
| Ade | d InForm | | | | | |
| | | | Cancel | | | |
| | | | | | | |

The new settings appear in the object section of the Q1 as:

- > OBJ, TYPE, INLET
- > OBJ, INFSRC_P1, den1*14*(xg/xulast
 - +yg/yvlast) with area
- > OBJ,INFSRC_W1,14* (xg/xulast+yg/yvlast) with onlyms

This is entirely equivalent to the settings

save13begin

(source of p1 at object is den1*14*(xg/xulast +yg/yvlast) with area)

(source of w1 at object is 14*(xg/xulast+yg/yvlast) with onlyms) save13end

There are advantages to this object-related method. Primarily, if the object is copied, the Inform statements will also be copied. If the object is renamed, the sources will still apply to the current object under its new name. The older method would require the InForm commands to be edited to match the new name, or copied for the new objects.

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4) PHOENICS Case Studies

4.1 PHOENICS modelling of the 'Dead Water' Effect Dr R P Hornby

During his epic voyage (1893-1896) to reach the North Pole in a specially designed boat (FRAM) with a hull strong enough to withstand pack ice pressure, the Norwegian explorer Fridtjof Nansen noted some peculiar behaviour of his vessel:

'moving at 5 knots, when the speed suddenly dropped to 1 knot and stayed that way'; 'we swept the whole sea along with us'; 'the moment the engine stopped, it seemed as if the ship was sucked back'.



Figure 1. Ship generating internal waves on the interface between deep dense water and less dense surface water.

These effects were later shown to be due to internal wave generation (see figure 1). This is particularly pronounced in highly stratified water (Norwegian fjords, for example) when the boat speed is similar to the phase velocity of excited internal waves. When the lower, dense, water depth is much greater than the upper depth of lower density surface water, the internal wave phase velocity (in m/s) is about half the square root of the upper layer depth. So, in deep water, with an upper layer depth of 9m, the internal wave phase speed is about 1.5m/s. Mariners caught in this 'dead water' observed that the water surrounding the ship had a glassy look bounded by a turbid edge (see figure 2) and this was sometimes accompanied by a prolonged hissing sound.



Figure 2. Sketch of the observed 'dead water' sea surface around a sailing boat: a turbid edge followed by a relatively smooth surface.

Professor Leo Maas of the Royal Netherlands Institute for Sea Research has recently hypothesised (New Scientist, December 2008) that the dead water effect could be responsible for some drowning incidents. In effect, swimmers swimming in stratified waters (deep lakes in summer, fjords, river outflows into the sea) could find a significant percentage of their propulsive power used to generate internal waves rather than forward motion – resulting in fatigue and drowning.

In order more clearly to understand the dead water effect, a series of experiments have been conducted at the Royal Netherlands Institute for Sea Research, starting with model boat experiments and culminating with experiments comparing swimming times in homogenous and stratified water. PHOENICS is being used to model these flows and compare with experimental results. Initially a 3-D transient model has been developed which couples the boat motion (determined by the boat propulsive thrust and the fluid drag) to the fluid flow. Figure 3 shows a comparison between the PHOENICS predictions and the experiment (which lasted about 20s) for a 'rectangular' boat shape.



Figure 3. Comparison of experiment (top) at 13.33s and the PHOENICS simulation at 13s for a rectangular boat shape. In the experiment the upper less dense layer is dyed red and overlays denser fluid (no dye). In the PHOENICS simulation the less dense fluid is coloured blue and the dense fluid coloured red. The boat is travelling from left to right.

The **PHOENICS** result is very encouraging, illustrating the essential interfacial wave characteristics well.



Figure 4. Predicted surface velocity vectors (colour coded) showing the presence of bow and stern, near transverse, attached, internal waves.

A full scale simulation has also been carried for a 56m length, 5m beam, 3.8m draft vessel with a displacement of 1000 tons moving at 0.9m/s in open water with an upper layer depth of 4m. For this case a wave absorbing region has been incorporated on the extremities of the lateral boundary to avoid non-physical wave reflections. The results for the surface velocity vectors are shown in figure 4. The principal features are attached, near transverse, bow and stern internal waves.



Figure 5. Close up view of near field surface flow vectors (colour coded) showing circulations of opposite sign in the bow and stern internal waves.

Figure 5 shows a close up of the near field surface velocity vectors showing that the waves at bow and stern have opposite circulation. This means that the region between these waves is a region of flow divergence which will tend to suppress surface waves. This is a possible explanation for the observed 'glassy' surface. Also the flow convergence at the head of the bow internal wave will promote surface waves which in certain circumstances may break causing a 'hissing' sound.

Future work will firstly concentrate on the effect of background internal waves on the boat motion. Ultimately, the flow created by a swimmer will be modelled using some of the more advanced **PHOENICS** features and results compared with the experiments at the Royal Netherlands Institute for Sea Research.

Dr R P Hornby e-mail: <u>bob@hornby007.wanadoo.co.uk</u>

CETIAT

Dr Eric Georgin (CETIAT–Villeurbanne–France) & Dr Jalil Ouazzani (Arcofluid–Pessac– France)

The LNE-CETIAT is the French expert in humidity. In order to calibrate instruments in all conditions, its laboratory is equipped with a humidity generator which produces moist air at the desired dew or frost point. Thermodynamically, the dew point is the temperature to which moist air must be cooled, at constant pressure, to condense water vapour into liquid water, ie dew. The frost point corresponds to almost the same definition except that ithe temperature is below zero and the condensed water is solid. Thus, dew or frost points correspond to an equilibrium state, at constant pressure and constant temperature, between the partial pressure of a moist air and liquid water or solid water, ie ice.

To improve its global knowledge about the humidity generator, the LNE-CETIAT, started a study about evaporation and condensation phenomena in its humidity generator. For this purpose we used the PHOENICS software on-line version. Thanks to this opportunity we constructed a preliminary model concerning the basic situation of pool boiling where a sheet of water is in contact with air in a cylindrical closed vessel. The transient state of mass and heat transfer was mainly studied.

Thanks to the "InForm" module, which allows users to add builtin equations, we implemented a large set of temperature-and pressure-dependent variables such as: air viscosity, air thermal conductivity, air heat capacity, saturation pressure, Fickian coefficient, etc. This on-line evaluation with the help of ArcoFluid, the CHAM representative in France, was really helpful in order to get an overview of PHOENICS capabilities even if we can not use the in-depth possibilities such as "ground".

In conclusion, we have decided to continue the modelling of our evaporation/condensation with the PHOENICS software.

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5) Consultancy Project Highlights Paul Emmerson

5.1 CFD Service AB



Figure 1 Vectors and velocity iso-surface of jet fan installation in a tunnel CHAM recently completed several projects with this company involving fire and ventilation analyses. A number featured modelling smoke movement from fires in underground tunnels and stations. The use of jet fans to control and limit the spread of smoke to aid evacuation of the tunnels is an important aspect of the analyses. CFD was used to optimise the positions of the jet fans. How the jet fans are installed is important, and can reduce their effective thrust output. Different scenarios were modelled to predict the jet velocity flow patterns in a standard-sized tunnel and hence ascertain "installation factors", which will be useful when considering different design configurations.

Other projects simulated flow of air in and around buildings and sports stadia. One interesting example analysed airflow within a circular hall, and required a redesign of the existing ventilation system to improve the thermal comfort levels. A number of different options were modelled so the optimum one could be taken forward and implemented.

5.2 Kirksey, Houston, USA, Natatorium Ventilation



Figure 2 Iso-surface of water vapour over swimming pool

Two steady-state simulations of a natatorium were carried out for Kirksey, an architecture firm based in Houston, to analyze flow, temperature and humidity for best and worst case wind scenarios with a combination of natural and forced ventilation. Thermal comfort parameters (Predicted Mean Vote and Predicted Percent Dissatisfied) and indoor air quality parameters - mean age of air were also analyzed.

The main area of interest was in the natatorium, but wind distribution external to the building was important to capture natural ventilation through doors and roof vents. A 3D-Studio engineering CAD file was imported into PHOENICS/FLAIR via AC3D, and the major features of the natatorium were included in the model. Each building component (eg walls, roof, beams etc) was separated into different geometry files to enable their material properties to be prescribed.

A number of open doors allowed natural ventilation into the building, together with gravity ventilation hoods on the roof modelled using a static pressure drop based on manufacturer's specifications. A system of exhaust vents was connected to a duct below the roof apex, driven by two fans provided mechanical ventilation. One of the scenarios included additional exhaust and inlet ventilation fans on the two main walls.

The calculation domain was extended far enough away from the natatorium building that pressure disturbances were not too close to fixed pressure boundaries. The "WIND" object was used automatically to set up wind profiles at upstream boundaries (specifying a wind speed/direction at a reference height and the power law to vary speed with height) and fixed pressure conditions at the sky and downstream boundaries.

Thermal material properties for walls and roof were specified, together with typical heat transfer coefficients. Incident solar radiation levels were prescribed on roof and walls taking into account reflection, absorption and radiation losses.

Water evaporation from the swimming pool was calculated from a standard ASHRAE correlation based on experimental data. The correlation considered local air velocity over the water surface, saturation vapour pressures at the water temperature and air dew point, and the latent heat of water at the pool temperature. The calculated mass of water evaporated from the pool was solved as the CFD calculation progressed, and was dependent on the predicted air conditions local to the pool. The mass of water was added as a source term to the cells next to the pool surface.

The calculation mesh had a total of 7 million grid points, with the majority in the region containing the natatorium. This provided sufficient refinement to resolve the geometry adequately and capture flow detail within the natatorium. The modified K- ϵ model of Chen and Kim was used to represent turbulence.

Both simulations were used successfully to assess whether natural and/or mechanical ventilation were feasible for best- and worst-case wind scenarios. Predicted temperatures, humidity levels and thermal comfort parameters were checked against target levels. The detailed predicted-air-flow patterns were analysed and used to redesign the position of exhaust and intake ducts to provide better comfort conditions.

6) Agent News

6.1 ACFDA Report Vladimir Agranat Gas Release& Dispersion CFD Module for Predicting Transient Flammable& Polluting Gas Clouds

In many industries, there are serious safety concerns related to the use of flammable gases in indoor and outdoor environments. It is important to develop reliable methods of analyses of flammable gas release and dispersion (GRAD) in reallife complex geometry cases. Computational fluid dynamics (CFD) is considered as one of the promising cost-effective approaches in such analyses. Over the last 6 years, the authors have been collaborating in CFD modelling of GRAD processes. As a result, the advanced robust CFD models have been developed, tested, validated and applied to the modelling of various industrial reallife indoor and outdoor flammable gas (hydrogen, methane, etc.) release scenarios with complex geometries. The user-friendly GRAD CFD modelling tool has been designed as a customized module based on PHOENICS.



Figure 1. Geometry and sensors for subsonic helium release in a garage

Advanced CFD models include the following: the dynamic boundary conditions, describing the transient gas release from a pressurized vessel, the calibrated outlet boundary conditions, the real gas law properties applied at high-pressure releases, the special output features and the local adaptive grid refinement (LAGR) tools. The predictions of transient 3D distributions of flammable gas concentrations have been validated using the comparisons with available experimental data. The validation matrix contains the enclosed and non-enclosed geometries, the subsonic and sonic release flow rates and the releases of various gases, e.g. hydrogen, helium, methane, etc. GRAD CFD module is recommended for safety and environmental protection analyses. It has been extensively applied to the hydrogen safety assessments including the analyses of hydrogen releases from pressure relief devices and the determination of clearance distances for venting of hydrogen storages. In particular, the dynamic behaviours of flammable gas clouds (with the gas concentrations between the lower flammability level (LFL) and the upper flammability level (UFL)) are accurately predicted with this module, which could be considered as a cost effective and reliable modelling tool for environmental assessments and design optimizations of combustion devices. The review paper¹ details the module features and provides currently available testing, validation and application cases relevant to the predictions of flammable gas dispersion scenarios.

A summary of this paper can be obtained from the authors.

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6.2 Arcofluid report Jalil Ouzani

a) Dr M. Antoni of University Paul Cezanne (Marseille, France) has been involved in the last year in modelling the movement of a liquid droplet in another liquid using the SEM method. He has improved the method by including through ground coding <u>surface tension</u> following Brackbill's work. He has been successful in reducing the diffusion around the droplet. His work is oriented towards emulsion. b) Dr. R. Adoua of University of Bordeaux (Wine Laboratory) has been conducting experiments and numerical modelling concerning the aging of wine in cylindrical vessels. He used the two phase models of PHOENICS (IPSA and Algebraic slip) successfully to reproduce accurately the experimental results.

c) Dr. Carrau of Fasis has been involved in the use of PHOENICS to study accidental risk, mainly the leak of propane in the atmosphere. He has been able to model the evaporative jet under strenuous conditions using the IPSA model.

d) Dr. E Georgin of Cetiat (Lyon, France) has successfully applied <u>INFORM</u> to account for evaporation of water through complex thermodynamics laws. (See his report).

e) Prof Emilia Crespo of UNED (Madrid, Spain) is using PHOENICS to study non-linear bifurcations occurring in cylindrical containers with low and high plates rotating. She studies particularly the departure from the axi-symmetric regime to a fully non axi-symmetric regime depending on non dimensional numbers based on cylinder dimensions, speed of rotation and amplitude of gravity.

f) Professor G. Sharan of Indian institute of Management in Ahmadabad has been using PHOENICS to optimise dew condensers; he is using the condensers passively to collect dew in the Gujarat region of India. Prof Sharan is very active in this field and has received many distinctions as well as a prize from UN related to his work. The principle for optimisation is to calculate the cooling down through radiation of special materials exposed to a clear sky. By using the PHOENICS code he is able to optimise the inclination and size of the condensers.



7) Technical Support

7.1 PHOENICS-FLAIR Mike Main

PHOENICS-FLAIR is used extensively for fire-engineering simulations with the support of CHAM's Technical Support engineers since the release of PHOENICS-FLAIR 2008.

The simplest treatment of a fire is to specify the heat release rate at the fire source over a pre-defined location and volume. PHOENICS 2008 introduced new menu panels for this purpose in terms of the FIRE object and "smoke-mass-fraction" settings. FLAIR utilises these new panels for newly-constructed cases, but the old menu panels can always be reinstated by setting the stoichometric coefficient to 0.0 under "Menu">"Models">"Smoke mass fraction settings"; and then from the main taskbar of the VR Editor (VRE), clicking on "File">"Save working files". The user must then enter fire, smoke and visibility data in the old menu panels to revert to the input system used in PHOENICS 2006 & PHOENICS 2007. If users read an old Q1 file into PHOENICS 2008 the VRE will retain the old menu panels for the fire object and smoke settings.

The first action for defining the fire and smoke model is to click "Menu">"Models" from the VRE, and activate solution of the conservation equation for the mass fraction of smoke as products of combustion (SMOK). Then click "smoke-mass-fraction" settings to bring up a new menu panel to specify heat of combustion H_{fur} , particulate smoke yield Y_s, stoichometric ratio R_{ox} , and specific extinction coefficient K_m. Next, the user defines location and size of the FIRE object, followed by specification of heat release rate, usually by means of the "Heat source table" provided by the heat-source option "piece-wise linear in time." It remains to specify the mass source of SMOK as "mass related." In the absence of using a

thermal radiation model, such as IMMERSOL, the FIRE objects define the convective heat release rate only, so the user is advised to set Hfu to $(1-X_r)^*$ Hfu, where X_r is the radiative fraction given, typically, as $X_r = 0.34$ in most fire-engineering handbooks. This practice ensures that the smoke generation rate will be computed from the total heat release rate, and not from the convective heat release rate.



In the current version, InForm should be used to compute smoke optical density. The relevant command is (STORED of SMOD is ODEN/5.29), which can be inserted into the Q1 input file by means of the InForm Editor in the "Menu">"Models" sector of the VR Editor. PHOENICS-FLAIR will write field values of the smoke optical density SMOD in units m⁻¹ to the PHI and RESULT files.

Also, in the current version users are advised to use an INLET object to define the volumetric extraction rate when a FAN object is located on a solution-domain boundary.

The technical support team have investigated a number of transient-fire simulations submitted by users and it appears that several such computations have been performed with an insufficient number of iterations (sweeps) for adequate convergence at a each time step. As explained in the PHOENICS documentation, there are three main tools that can be used to determine whether reasonable convergence has been achieved, namely overall source balances, absolute residual behaviour, and monitor spot value behaviour or maximum correction behaviour.

Despite the presence of a very large mesh, values as low as 10 sweeps per time step have been observed, whereas typically, values ranging from 50 to several hundred sweeps may be required for adequate convergence, depending on the size of the time step, the temporal nature of the boundary conditions and heat release rate, and also on whether jet fans or other such devices has been activated suddenly at some stage in the transient. For the first few time steps, as many as 2000 sweeps may be required, especially if the initial flow field is stagnant and ventilation units are activated at the first time steps. In these cases it might be expedient to initiate the transient run from the solution fields produced by a steady-state precursor CFD simulation. Another point to note is that, generally speaking, the smaller the time step the more accurate the solution, and the less sweeps required for adequate convergence. However, for large industrial applications, the use of too-small time steps may prove impractical because of the computer time required to cover the transient of interest.

Users are strongly advised to check convergence at each time step, so that numerical errors are not transmitted to later time steps, producing inaccurate solutions, and sometimes perhaps implausible flow fields. A particular example was observed for a fire in an underground car park. An insufficient number of sweeps led to incomplete convergence and, consequently, a CFD solution which failed to predict smoke backlayering along the ceiling of the car park. When the computation was repeated with a sufficient number of sweeps, the simulation predicted smoke rollback along the ceiling because in the converged state, the fireinduced buoyancy forces overcame the inertial forces of the ventilation in the ceiling layer.

8) News and Events 2009

Courses and Meetings



Dr Jeremy Wu delivered a PHOENICS/FLAIR training course April 15-17 at ZEB Technology in Singapore following the basic threeday programme with extra workshop time. Participants worked interactively on screens to complete cases and share experiences, explanations could be added and interactions were instant. Participants could use default grid settings behind the scenes to get results without needing to set up individual grids; they used grid generation combined with PARSOL which they found easy to follow and use. Participants brought specific problems to the session and create models to solve those problems. If problems arise with model creation, Dr Wu could assist with required minor adjustments. The Course was a success and participants were impressed with what they were able to achieve.

| May 18-20 | Arcofluid Course at CETIAT in Villeurbanne |
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| June 1-6 | Global Energy Award Ceremony, St Petersburg, Russia. Professor Spalding receives the Global Energy International Prize for his work on heat and mass transfer and fluid flow. |
| Jun 5-7 | Shanghai Feiyi is participating at ISEC 2009 Exhibition in Shanghai <u>www.chinaisec.com</u> |
| Jul 21-23 | Next PHOENICS Training Course at CHAM: a regular CHAM Course comprising a <u>Three-day Introduction</u> . Attendees may come for only part of the time. e-mail <u>sales@cham.co.uk</u> to register for the next training course or to obtain further information. Courses can be run at customer sites by prior arrangement, see: <u>http://www.cham.co.uk/training.php</u> . |
| Aug 24-28 | Arcofluid is participating in the French Congress of Mechanics in Marseilles |
| Sep 21-23 | Arcofluid Course at the University of Bordeaux |

CHAM Staff News

We are pleased to announce that Dr Qin is back at CHAM full time after a recent bout of illness and that David Glynn has returned as an external consultant. We congratulate John Smith on reaching retirement age in May and are pleased to announce that he is remaining with CHAM.

CHAM Japan News

CHAM Japan was joined in February by Mr Yoshihiro Ishida who has worked with Itochu, Kanematsu Electronic, Toshiba Group, Nihon, Honda, and Sony. CHAM Japan has also moved into new, more extensive, offices.