PHOENICS News

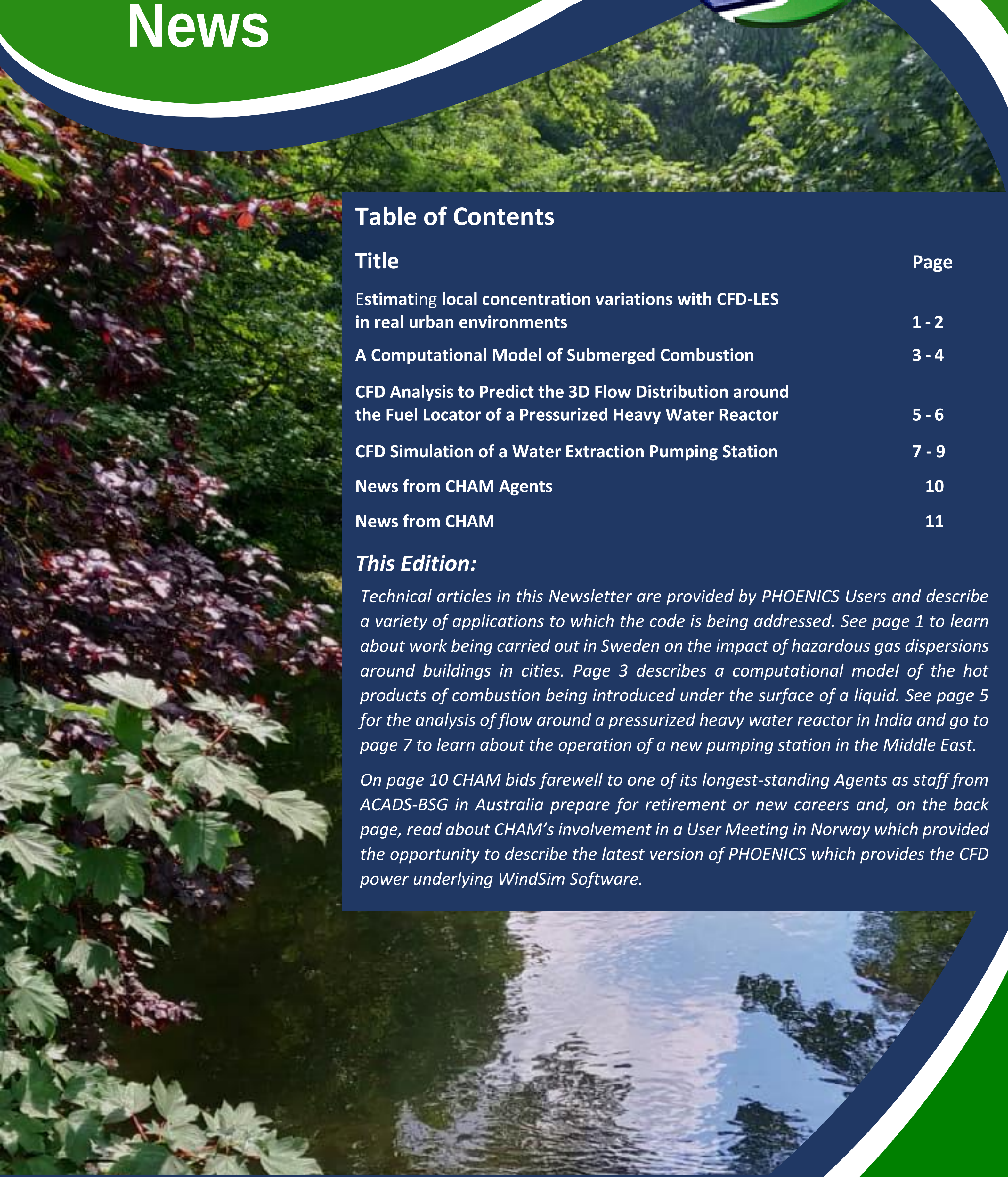


Table of Contents

Title	Page

This Edition:

Technical articles in this Newsletter are provided by PHOENICS Users and describe a variety of applications to which the code is being addressed. See page 1 to learn about work being carried out in Sweden on the impact of hazardous gas dispersions around buildings in cities. Page 3 describes a computational model of the hot products of combustion being introduced under the surface of a liquid. See page 5 for the analysis of flow around a pressurized heavy water reactor in India and go to page 7 to learn about the operation of a new pumping station in the Middle East.

On page 10 CHAM bids farewell to one of its longest-standing Agents as staff from ACADS-BSG in Australia prepare for retirement or new careers and, on the back page, read about CHAM's involvement in a User Meeting in Norway which provided the opportunity to describe the latest version of PHOENICS which provides the CFD power underlying WindSim Software.

Concentration Heat and Momentum Limited, Bakery House, 40 High Street, Wimbledon, London SW19 5AU, UK
Telephone: 020 8947 7651   Fax: 020 8879 3497
E-mail: phoenics@cham.co.uk, Web site: http://www.cham.co.uk

Summer 2019

Estimating local concentration variations with CFD-LES in real urban environments

Jan Burman,[1,3] Lage Jonsson,[*1,2] and Anna Rutgersson[3]

[1)] FOI, Swedish Defence Research Agency, Division of CBRN Defence and Security, SE-901 82 Umeå

[2)] KTH, Royal Institute of Technology, SE-100 44 Stockholm, Sweden

[3)] Department of Earth Sciences, Uppsala University, Uppsala, Sweden

Applied studies with Large Eddy Simulation (LES) of hazardous gas dispersion around buildings in cities have become increasingly feasible due to rapid advancements in computing technology. In this study [1], the potential of CFD-LES for these applications was investigated by using three typical LES sub-grid-scale (SGS) models in combination with either synthetic turbulence, or no turbulent fluctuations at inflow boundaries. Specifically, the Smagorinsky [2], WALE [3] and SIGMA [4] SGS models were used within the framework of the general-purpose CFD code, PHOENICS. The use of synthetic inlet turbulence [5] was restricted to simulations made with the SIGMA SGS model. To avoid excessive numerical damping of the predicted fluctuations, the 3rd-order implicit Adams–Moulton scheme was used for temporal differencing, and the bounded higher-order TVD scheme MUSCL was employed for discretisation of spatial convection. The PHOENICS cut-cell solver was used to represent the complex cityscape geometry on a background Cartesian mesh.

The CFD-LES model was applied to simulate the continuous-release IOP2 data set from street-canyon experiments performed under the Joint Urban 2003 Atmospheric Dispersion Study in Oklahoma City [6-10].

One of the objectives of these experiments was to collect flow and tracer concentration data at various distances from the release point, with a large number of wind and tracer sensors placed at both street and roof level.

Flow and turbulence statistics of CFD-LES were presented at two probe locations [1], one inside the city-core and one outside. In addition, comparisons were made with the measured mean concentration and maximum concentration values [1].

LES was carried out on the solution domain shown in Figure 1, which measures 800 × 850 × 300 m. An aerodynamic roughness length of 0.02m was specified for the ground terrain, and the wind logarithmic velocity profile was specified as (1.97m/s, 2.82m/s) at a height of 10m, with a roughness height of 0.6m. The tracer gas release rate for the experiments was 5g/s.

A mesh count of 218 × 272 × 100 cells was used with cell sizes in the streets typically about 1 m square. The index of resolution quality [11,12] for the LES was adequate for engineering purposes, and the simulation was advanced in time for 60s before initiating evaluation of all flow variables and spectra.

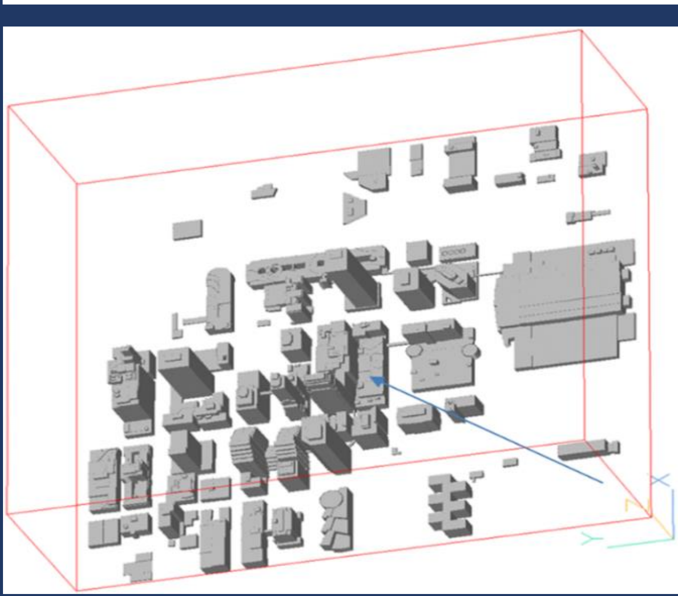


Figure 1. Solution Domain for JU2003 Experiment. The arrow indicates the main wind direction.

The complete set of results, including comparisons between the field measurements and simulations of the gas-dispersion characteristics, has been reported in detail elsewhere [1. Some typical results are shown in Figure 1, which illustrate the predicted gas dispersion by contour plots taken at 2m above ground level, and overlaid by surface plots at 0.25 mg/m^3 from the continuous source (IOP2), 150s after initiation. The results were obtained by the SIGMA SGS model with no inlet fluctuations.

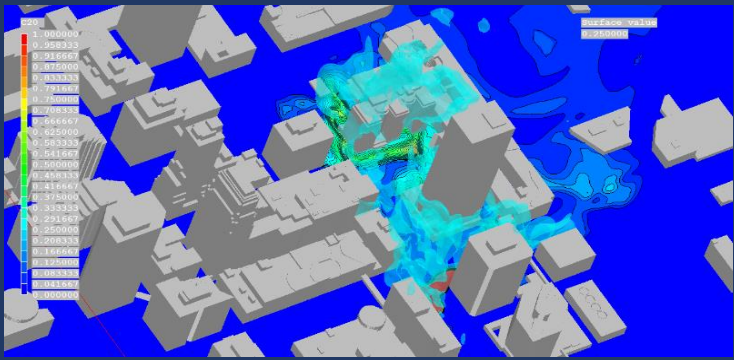


Figure 2. Tracer dispersion contours at ground level (2m).

In summary, it was found that, in the core of the city, simulated turbulence was mainly determined by buildings and their configurations, and was only weakly affected by the type of SGS model and assumed turbulence at inflow boundaries. On the other hand, outside and upwind of the city centre, turbulence specified at the inflow boundaries was very important if realistic turbulence statistics were to be achieved. Downstream of the source, all tested models produced similar predictions of maximum concentration values, which in turn were similar to experimental data.

References

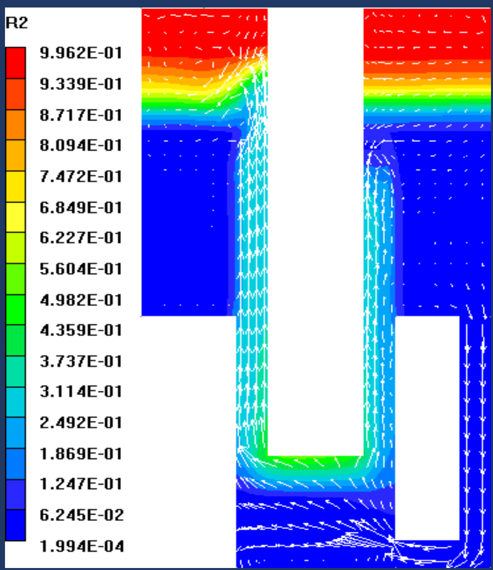
1. Burman, J., Jonsson, L., Rutgersson, A.: On possibilities to estimate local concentration variations with CFD-LES in real urban environments, Environmental Fluid Mechanics, Vol.19, No.3, 719-750, https://link.springer.com/article/10.1007/s10652-018-9650-4, (2019).
2. Smagorinsky, J.: General circulation experiments with the primitive equations. Mon. Weather Rev., 91:99–164, (1963).
3. Nicoud, F., Ducros F.: Sub-grid-scale stress modelling based on the square of the velocity gradient tensor flow. Turbulent Combustion, 62:183–200, (1999)
4. Nicoud, F., Baya, H.T., Cabrit, O., Bose, S., Lee J.: Using singular values to build a sub-grid-scale model for large eddy simulations. Phys Fluids 23:085106, (2011).
5. Davidson, L.: Using isotropic synthetic fluctuations as inlet boundary conditions for unsteady simulations. Adv Appl Fluid Mech 1(1):1–35, (2007).
6. Garvey, D., Bustillos, M., Chang, S., Cionco, R., Creegan, E., Elliott, D., Huynh, G., Klipp, C., Ligon, D., Measure, E., Quintis, D., Torres, M., Vaucher, G., Vidal E., Wang, Y., Williamson, C., Yarbrough, J., Yee, Y.: U.S. army research laboratory meteorological measurements for joint urban 2003. Army Research Laboratory, Adelpi, ARL-TR-4989, (2009).
7. Nelson, M.A., Pardyjak, E.R., Klein, P.: Momentum and turbulent kinetic energy budgets within the Park Avenue Street Canyon during the joint urban 2003 field campaign. Boundary Layer Meteorology, 140:143–162, https ://doi.org/10.1007/s1054 6-011-9610-8, (2011).
8. Allwine, K.J, Flaherty, J.E.: Joint urban 2003: study overview and instrument locations. Pacific Northwest National Laboratory, PNNL-15967, (2006).
9. Clawson, K.L., Carter RG., Lacroix, D.I., Biltoft, C.A., Hukari, N.E., Johnson, R.C., Rich, J.D., Beard, S.A., Strong, T.: JOINT URBAN 2003 (JU2003) SF_6 atmospheric tracer field tests. Air Resource Laboratory, Silver Spring, Maryland, NOAA technical memorandum OAR ARL-254, (2005).
10. Leach, M.J.: Final report for the joint urban 2003 atmospheric dispersion study in Oklahoma City: Lawrence Livermore National Laboratory Participation, UCRL-TR-216437, (2005).
11. Celik I.B., Cehreli, Z.N., Yavuz, I.: Index of resolution quality for large eddy simulations. J Fluids Eng. T ASME 127:949–958. https ://doi.org/10.1115/1.19902 01, (2005).
12. Celik, I., Klein, M., Janicka, J.: Assessment measures for engineering LES applications. J Fluids Eng. T ASME 131:1–10, (2009).

A Computational Model of Submerged Combustion

By S.V. Zhubrin, Independent Researcher, svzhubrin@yahoo.co.uk

Submerged combustion [1] is a process where the combustion of gas or liquid fuel releases the hot products of combustion *under* the surface of a liquid or melt. This has the advantage of achieving maximum heat transfer rates by direct contact of the combustion gases with the liquid or melt. Industrial applications of the technology exist in two main areas. The first concerns liquid heating and/or evaporation using submerged-combustion devices (SCDs). The second uses submerged-combustion melters (SCMs) for hazardous waste treatment, melting silicate materials, producing mineral wool, glass manufacturing etc. in melting technologies. SCMs are always arranged with a burner submerged into or beneath the melt, whereas SCDs mostly employ the burner above the liquid level with a submerged exhaust system.

An Eulerian-Eulerian two-phase CFD model of submerged combustion (SUBCo) has been developed within PHOENICS for industrial applications. The model uses idealization of interpenetrating continua to provide a mathematical description of the behaviour of liquid and fragmented within-liquid gas phases with full account taken of momentum, heat- and mass transfer between phases. The latter takes place between the usually colder liquid phase and the submerged hot gaseous products of combustion. The local volume occupancy of each phase is defined by the phase volume fraction obtained from the solution of its own conservation equation.

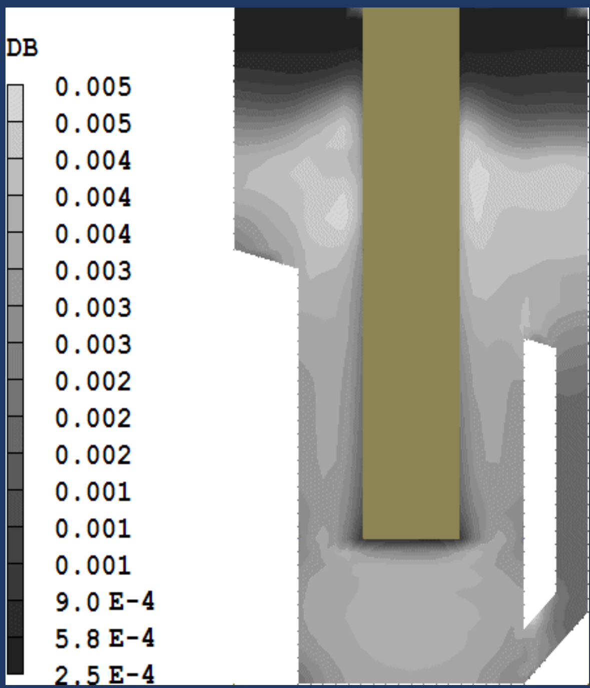


Water circulation vectors and gas phase volume fraction contours in a gas-lift evaporator.

In its IPSA [2] embodiment, which is unique to PHOENICS, a volume-fraction equation is written for each phase. It involves: phase density, phase velocities, a diffusion coefficient to account for gas-phase turbulent dispersion; and mass exchange between each phase per unit time and volume. This represents evaporation and condensation processes. Phase volume fractions are also related to each other through the requirement that they sum to unity to satisfy overall continuity.

Conservation equations are also solved for a number of gas-phase variables, typically including: three velocity components, enthalpy and the mass fractions of all the major participating chemical species, and if necessary, minor ones for the pollutants. For the liquid phase, equations are solved for the three velocity components, enthalpy and the mass fractions of all liquid components. All of these conservation equations have a similar form to the phase volume-fraction equations, but with additional terms representing turbulent diffusion and inter-phase transfer processes, such as for example those associated with the exchange of mass, momentum and energy. There are also within-phase sources in these equations, including those concerned with the rates of exothermic chemical transformation of the fuel-air gas phase mixture into gaseous combustion products. The latter are generated by within-gas chemistry-turbulence interactions represented by the eddy dissipation approach. Two turbulent diffusion terms are featured in the conservation equations; one is responsible for the exchange of conserved property through turbulent diffusion of a phase, and the other is the within-phase turbulent diffusion.

To calculate turbulent transport, both phases are assumed to share the same mixture turbulent viscosity and corresponding diffusion coefficients [3]. The value of the mixture turbulent viscosity is calculated as the volume-fraction average of phase-stream turbulent viscosities, which are calculated via the phase absolute velocities and the distance to the nearest wall. The latter is computed from the distance-function differential equation taking into account the arrays of any sub-cell solid inserts [4]. The field distribution of dominating gas-phase fragment sizes, in a gas-liquid flow with phase inversion, are computed using a constitutive relation for the inter-phase momentum transfer [5], and a model based on the equilibrium limit of the transport equation for fragment size [6,7]. The latter allows for size diminution and enlargement due to mass transfer, and for other mechanisms which may cause a fragment-size change, such as gas breakup and/or coalescence.



Contours of gas-fragment size

The present contribution has described how the IPSA solver of PHOENICS can be converted into an efficient computational tool which allows the calculation of the momentum, heat and mass transfer, as well as the chemical and phase-change transformations for the technology of submerged combustion. The developed methodology can readily incorporate further combustion sub-models with advanced turbulence-chemistry and radiation interactions, such as the Stream Recognition Model [8], and gas-fragment-size evolutions, for instance those in which gas-phase fragmentation is influenced by the local gas-liquid population balances.

References

1. Collier, J.G.: Submerged combustion, http://www.thermopedia.com/content/1164/ (2011).

2. Spalding, D.B.: Numerical computation of multi-phase flow and heat transfer. Contribution to: 'Recent Advances in Numerical Methods in Fluids. P139-167, Eds. C.Taylor & K.Morgan, Pineridge Press, Swansea, UK (1980) (see also http://www.cham.co.uk/phoenics/d_polis/d_lecs/ipsa/ipsa.htm).

3. Zhubrin, S.V.: Zero-equation turbulence model for gas-liquid simulations, July 2006, https://dx.doi.org/10.13140/RG.2.1.4558.5442

4. Zhubrin, S.V.: Computations of wall distances for distributed resistance analogy, August 2015, https://dx.doi.org/10.13140/RG.2.1.4845.5524

5. Zhubrin, , S.V.: Inter-phase Momentum Transfer for Phase Inversion Conditions, July 2004, https://dx.doi.org/10.13140/RG.2.1.4578.5125

6. Agranat, V.M., Zhubrin, S.V., Maria, A., Kawaji, M.: Gas-liquid flow analyser for water electrolysis, March 2006, https://dx.doi.org/10.13140/RG.2.1.3044.5605

7. Zhubrin, S.V.: An algebraic fragment-size model for gas-liquid flows with phase inversion, November 2007, https://dx.doi.org/10.13140/RG.2.2.17697.66400

8. Zhubrin, , S.V.: Development of stream recognition model of transported probabilities for turbulent flames, January 2018, https://dx.doi.org/10.13140/RG.2.2.30732.006

CFD Analysis to Predict the 3D Flow Distribution around the Fuel Locator of a Pressurized Heavy Water Reactor, by Jaspal Singh Bharj Nuclear Power Corporation of India Limited, Nabhikiya Urja Bhavan, Anushaktinager, Mumbai-400 094, India

A Pressurized Heavy Water Reactor (PHWR) has 392 coolant channels mounted horizontally, and each channel contains 13 fuel bundles, 2 fuel locators, 2 shield plugs and 2 sealing plugs. The two fuel locators are kept in the coolant channel, one at the upstream end, and one at the downstream end of the fuel string. The fuel locator, which is shown schematically in Figures 1 and 2, serves mainly to locate the shielding plug closer to the sealing plug. The heavy water entering the coolant channel flows in the annulus of the liner tube, which has a number of rows of peripheral holes through which the coolant passes radially. In order to avoid undue vibration and fretting of the fuel bundle, the fuel locator converts this radial flow of heavy water to an axial flow parallel to the fuel bundles, which are located downstream. This conversion is facilitated by suitably tapering the front-section of the fuel-locator body; and, ideally, the design should produce a uniform flow distribution into the fuel bundle to avoid any flow-induced vibration. The design has been investigated by performing three-dimensional numerical simulations with the PHOENICS CFD software, the objective being to predict flow distribution over the fuel locator, and the flow profile at the fuel-locator exit. The complicated geometry of the fuel locator has been modelled in PHOENICS Version 2018 using the cut-cell solver on a cylindrical-polar co-ordinate mesh with a total of 5.824 million cells. The analysis has been carried out under isothermal and steady state conditions using the standard k-ϵ turbulence model. The modelled geometry considered for the study is shown in Figures 1 and 2.

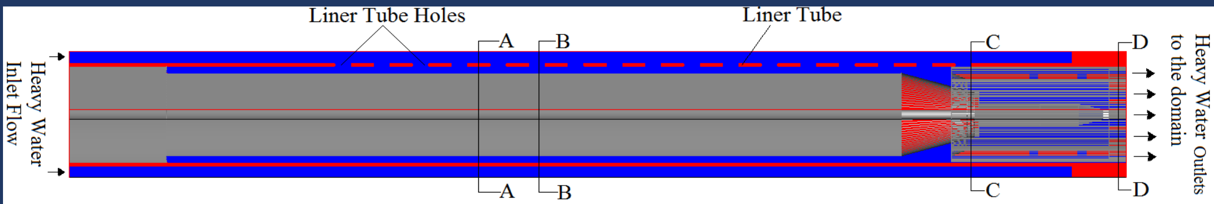


Figure 1. Modelled Geometry of the Fuel Locator in PHOENICS

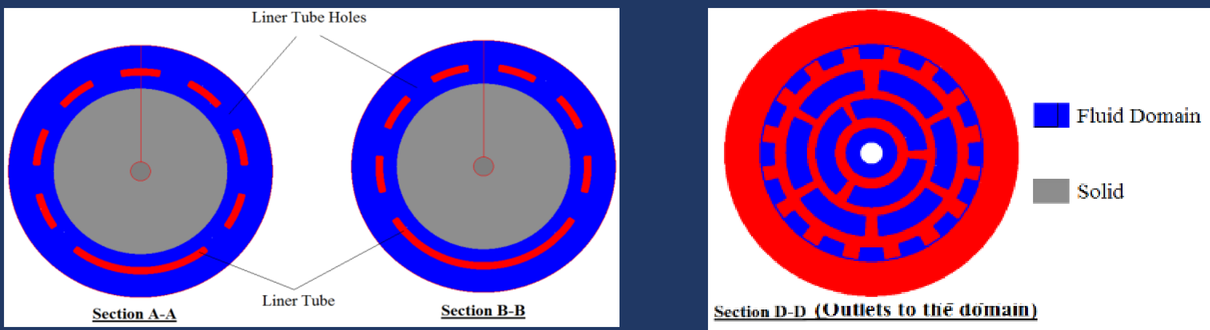


Figure 2. Section A-A, Section B-B and Section D-D

The results of the CFD study are presented in terms of absolute velocity contours inside the fuel locator. Figure 3 presents results for the central vertical plane through the fuel locator; and Figure 4 shows results for an enlargement of the circled region A shown in Figure 3, and for the cross sections C-C and D-D identified in the same figure.

. **Figure 3, Contours in the central vertical xial plane**

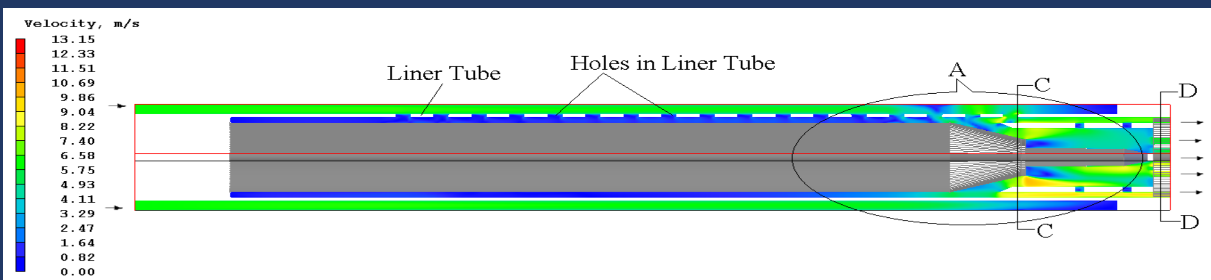
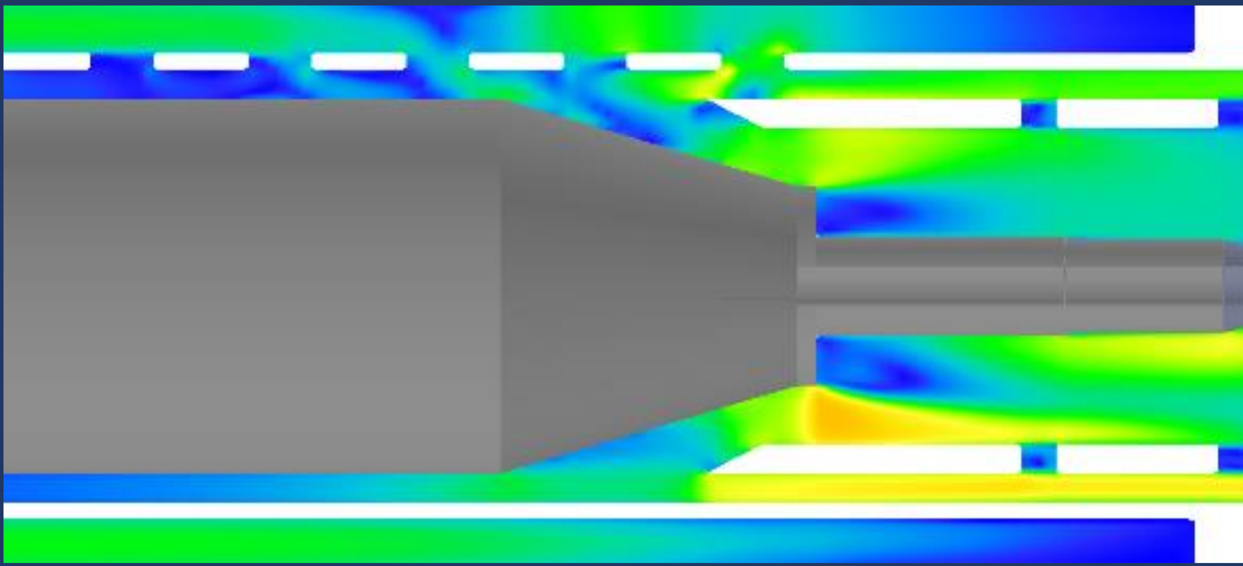
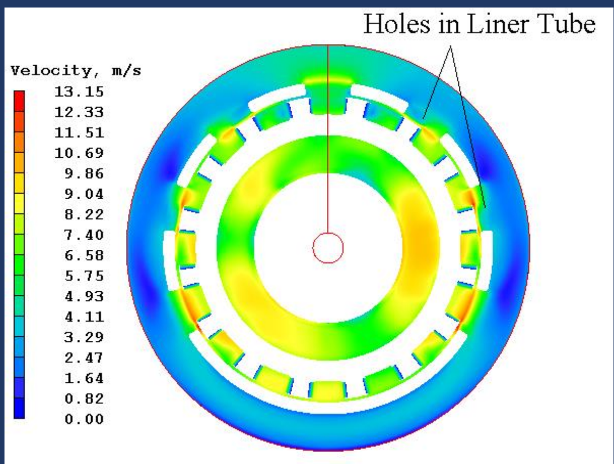
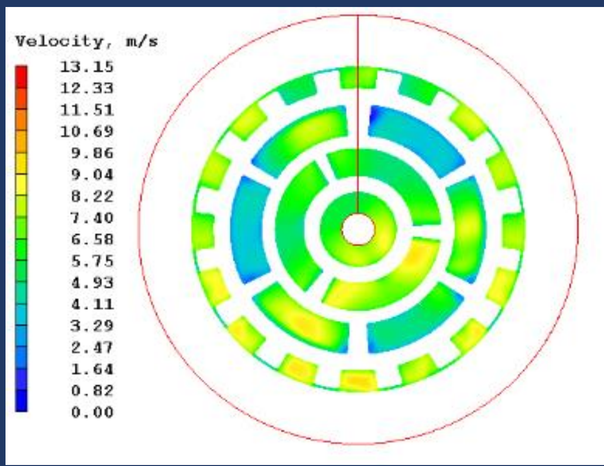


Figure Velocity contours in the central vertical axial plane.



View A





Section C-C **Section D-D** **(Through Outlets)**

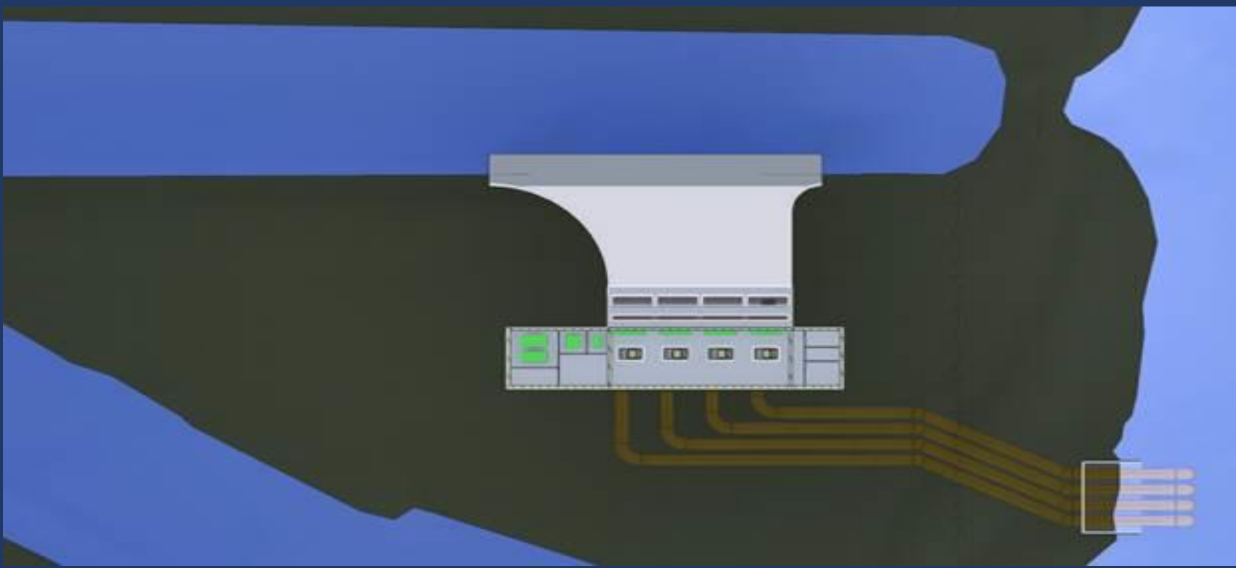
Figure 4. Velocity contours in the central vertical axial plane and Sections C-C and D-D

It is clear from the above velocity contours that the fluid enters the solution domain and flows in an annular direction over the liner tube (outer annular flow). Fluid then enters the locator region through the holes on the liner tube, with higher flow rates through the last few sets of holes relative to those further upstream. This is because there is no other route by which the remaining outer annular flow can escape into the locator region that leads to the outlets at the end of the domain. It can be seen from the velocity contours in section C-C of Figure 4 that the fluid enters the last set of liner tube holes with a peak local velocity of about 13 m/s. Here the flow is akin to the angled flow through an orifice plate, and separation occurs there as the flow accelerates past a sharp edge.

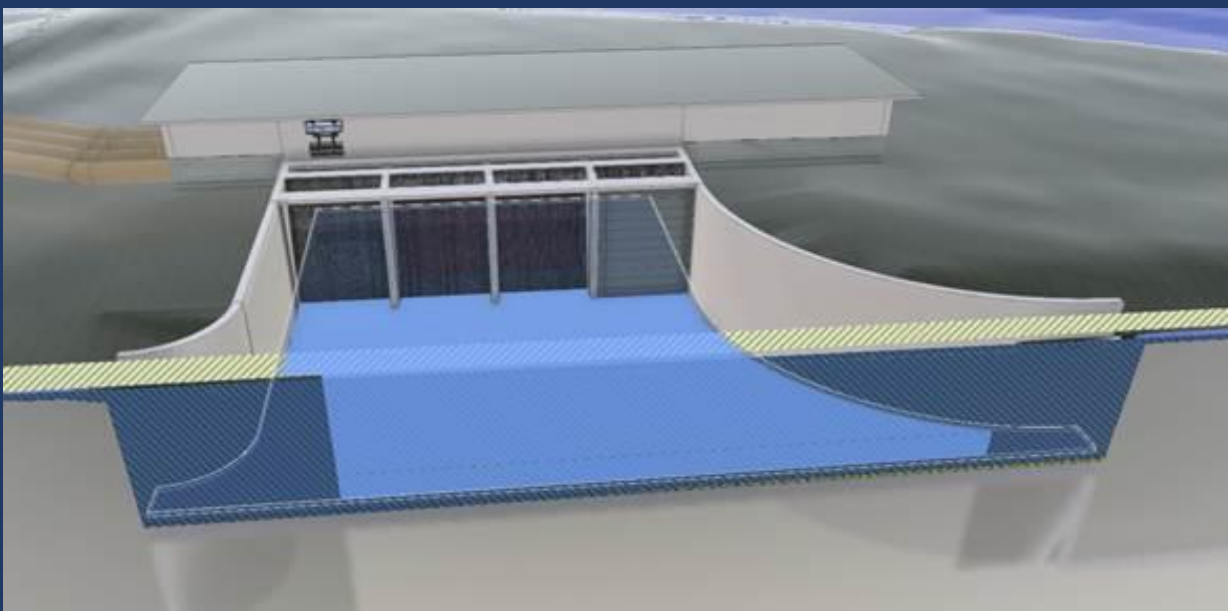
The CFD analysis has revealed that the tapered part of the fuel locator plays a significant role in guiding the coolant flow towards the central portion of the locator, resulting in an almost uniform distribution of the coolant velocity at the peripheral outlets (see section D-D in Figure 4). Thus, the fuel locator converts the radial flow of heavy water through the holes in the liner tube to an axial flow parallel to the fuel bundles in the channel. The almost uniform flow profile predicted at the exit means that the design should avoid any undue vibration and fretting of the fuel bundle.

CHAM Case Study – CFD Simulation of a Water Extraction Pumping Station by Timothy Brauner, CHAM & Katarzyna Bozek, RHDHV Scientist, Water Europe.

Haskoning DHV UK Limited, a division of the Royal Haskoning DHV Group, approached CHAM for assistance in predicting the operation of a new pumping station being designed for a planned development in the Middle East. The objective was to model water entering a pumping station from the approach channel/forebay, through an intake and past dividing walls that separate four pumps. Two orientations of the pumping station were considered; the first angled at 90^{o} to the channel, and the second angled at 30^{o}. The purpose of the exercise was to compare the two proposed designs by reviewing the 3D velocity field approaching the pumping station, through the intake bend and fine eel screens, and finally through separation walls to the pumps.

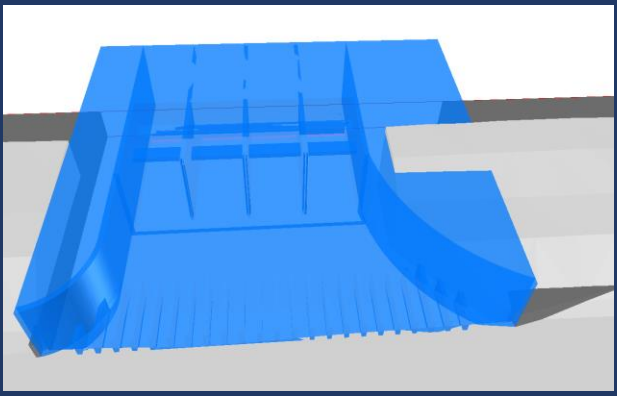


Pumping Station schematic Plan View

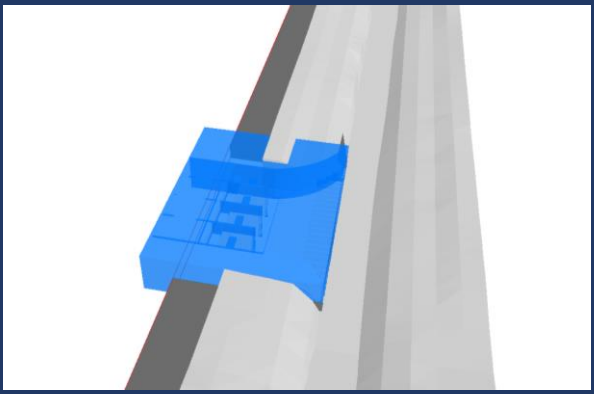


Pumping Station schematic with intake bend & eel screens

The CFD model was created using terrain data for the approach channel and CAD input for each pumping station orientation. Cases were run as single-phase, steady-state models, with the upstream water level and downstream pump capacity both fixed (and taken from other modelling data). The CFD model ended downstream of the pump intakes at four abstraction points before the pipes.



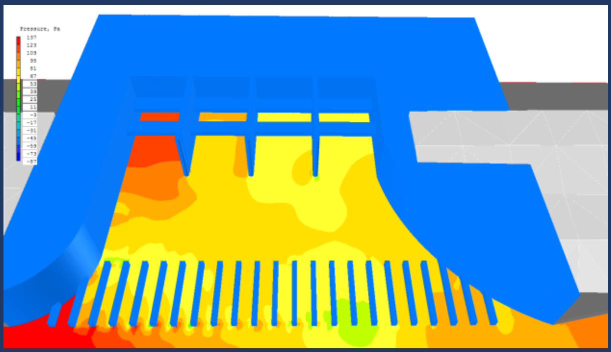
Pumping Station CAD import



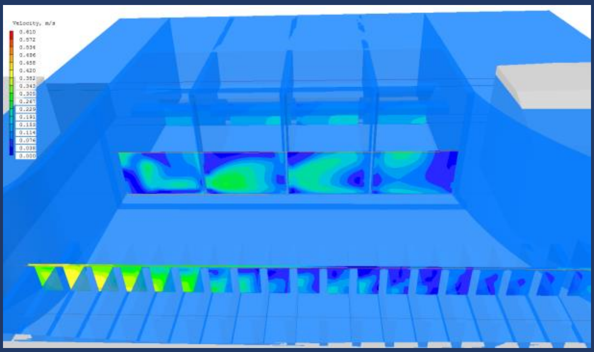
Pumping Station CAD import with approach channel

The initial case studied the water flow, without the eel screens in situ, using a grid of 800,000 cells. It took less than 2.5 hours to converge on a 3.4GHz quad-core PC with 16GB RAM.

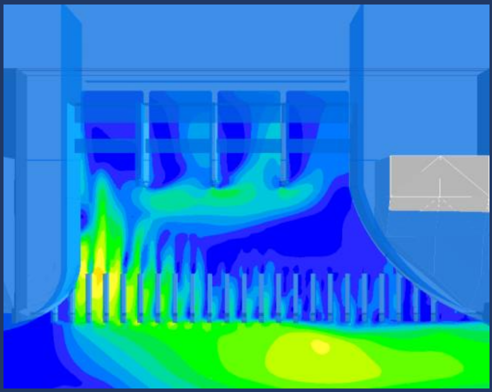
The result for the 90^{o} angle shows a not-unexpected imbalance in water pressure, and the velocity has been tempered only slightly by the preceding guide channels. The momentum of the water in the approach channel carries it past a large section of the pump station intake, resulting in the bulk of the water entering the station through the downstream baffles. The pumps, all operating at the same extraction rates, force the water to redistribute itself in the area between the baffles and the separation walls to the pumps, resulting in an uneven and circulating flow field.



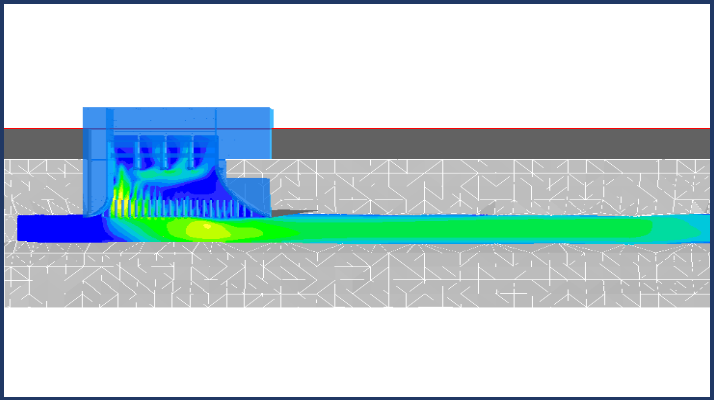
Pressure 0.9m depth



Velocity Y slices

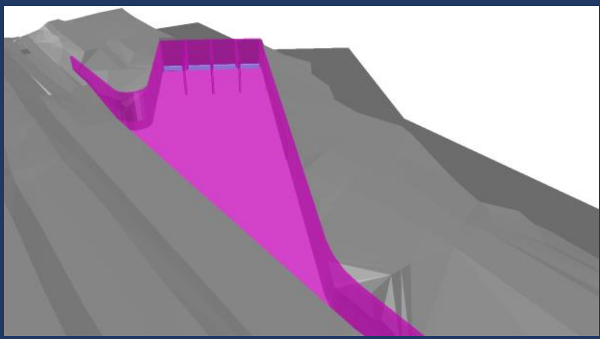


Velocity 0.9m water depth Plan View

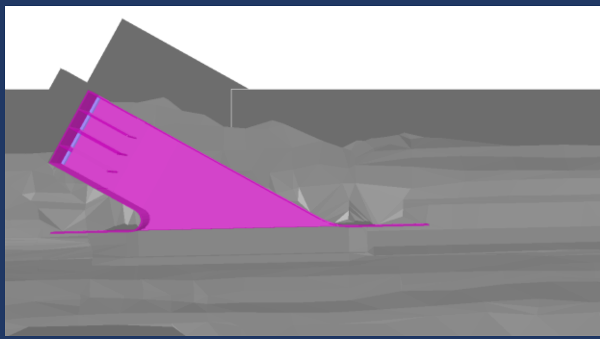


Velocity 0.9m water depth including approach channel

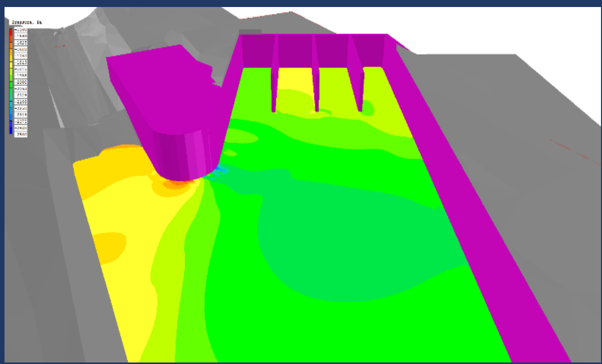
An alternative orientation for the pumping station to the channel was investigated; this involves a shallower, 30^{0} angle of the pump station to the channel, as shown below:



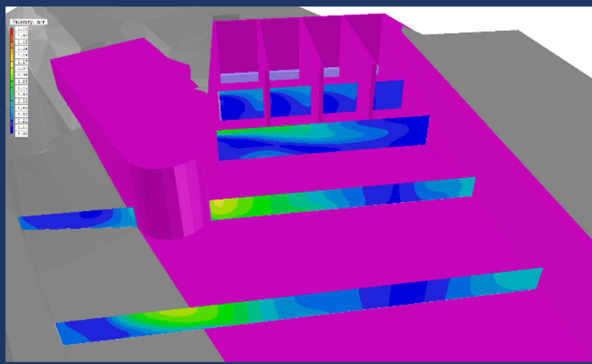
Pump Station re-positioned at 30 angle



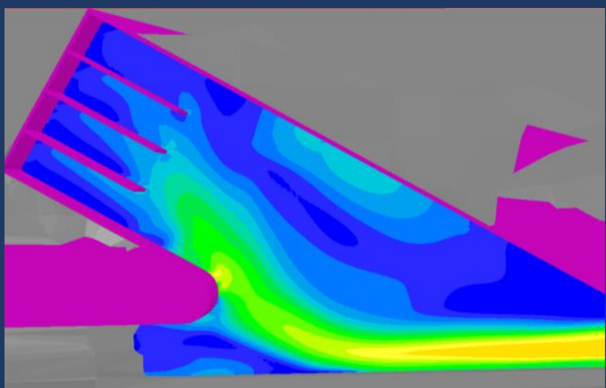
Velocity 0.9m water depth including approach channel



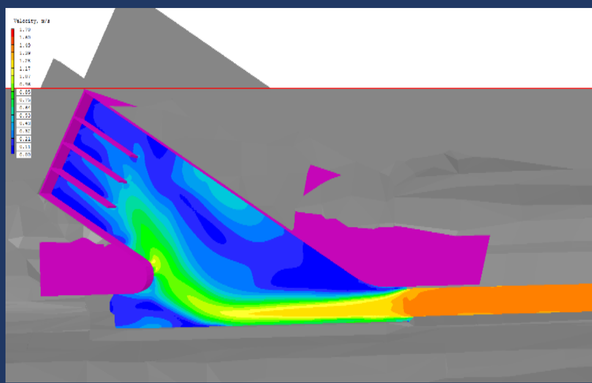
Pressure of water depth of 0.9m



Velocity Y slices



Velocity at depth 0.9m, Plan View



Velocity at 0.9m depth with approach channel

The preliminary 30^{0} rotated design proved to be only partially successful. The high-momentum water from the channel continues to travel along the same direction as the channel, and eventually turns into the pump station due to the pumps and a pressure build up in the overflow channel. This results in a large rotating region of water covering most of the pump station forebay.

This particular design did not employ guide vanes, as were installed in the previous CFD model. These were subsequently re-instated by the client and their curvature adjusted for optimum performance during their next stage of design investigations – once again demonstrating the cost- and speed- benefits of using trial-and-error CFD simulation ahead of physical modelling or full-scale construction.

News from CHAM Agents

It is with regret that CHAM announces the cessation of its Agency Agreement with ACADS-BSG based in Australia. ACADS became a CHAM Agent in 1995 and we have worked closely together ever since.

Murray Mason, with whom we have worked for the past 24 years, has turned 80 and his co-Director Trevor Kingston is 65. They have decided that this is the appropriate time to sell the company and enjoy a well-earned retirement.

ACADS-BSG came about when, in 1980, a Building Services Group (BSG) integrated as a division of a not for profit organisation called ACADS (The Association of Computer Aided Design). In 1994 it separated from ACADS and was set up as a separate company with the two names becoming one.

Initially when the building services group was set up within ACADS, two air-conditioning load-estimation programs and a duct design program were made available to a handful of users via a computer bureau. In those days they were DOS based. Copies of the programs were also licensed and supplied to users on magnetic tape. Since then ACADS-BSG has developed, or acquired a comprehensive range of building services programs, including software for piping and sprinkler systems design and energy simulation, and has been the agent in Australia, SE Asia and New Zealand for PHOENICS, FLAIR and other CHAM Products.

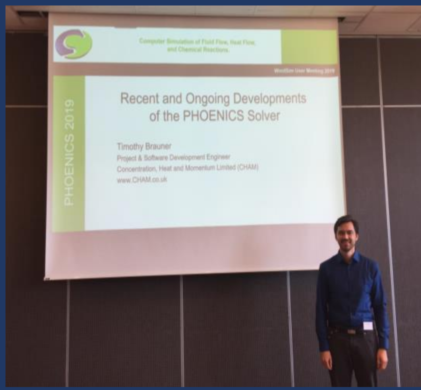
In 2004 ACADS-BSG ran the first and only PHOENICS User Conference in Australia, and in 2008 hosted a PHOENICS workshop in Sydney. It also regularly had a stand at the bi-annual ARBS (Air-conditioning, Refrigeration and Building Services) Trade Exhibition where PHOENICS has been demonstrated. At a Gala Presentation Dinner at ARBS 2012 Murray Mason was inducted into the ARBS Hall of Fame, in recognition of his significant contribution to the industry.

Murray, Trevor and other members of staff at ACADS-BSG have been part of the CHAM-PHOENICS family over the years and we will miss having them on board.

All at CHAM wish them well in their retirement and hope that they are able to spend their time doing whatever they wish without the necessity of concentrating on time in the office.

WindSim User Meeting 2019 Summary by Timothy Brauner

The 14th User Meeting took place on June 5 – 6 in Tønsberg, Norway and was attended by Dr Timothy Brauner from CHAM. The meeting comprised 1.5 days of presentations and workshops with a social event at the end of the first day. The conference was attended by representatives from 19 companies and 4 universities, as well as WindSim employees.



Day 1 started with a welcome by WindSim CEO Donna Rennemo, and CTO Arne Gravdahl followed by an update regarding recent and ongoing product development. The day was filled with presentations by users detailing use of, and experience with, WindSim software. Applications ranged from optimising wind turbine placement, power forecasting and modelling natural hazards, to more academic investigations of boundary layer models. The day was rounded off with three presentations by Masters' students who used WindSim for their thesis projects.

The social event involved a sailboat trip to and from the location where a dinner was held. There were 5 boats with 7 people and a skipper each. Our boat was crewed by Donna Rennemo, one of WindSim's software development engineers Tejo de Groot, representatives of EnBW Energie, METEOTEST, Suzlon Energy and myself. The dinner featured copious amounts of shrimp and wine and a 23:00h sunset.

Day 2 started with 3 presentations, including that from CHAM on recent and ongoing development work of relevance to software which will be offered by WindSim in the near future. The second half of the session offered 3 parallel workshops on Quality Managements Systems, Meso-Microscale Coupling and, the most popular of the sessions, Blockage Effects. WindSim are looking to incorporate this blockage effect upstream of wind farms in their new Actuator Disk Model.

The meeting was a good occasion to interact with users and hear their feedback. Users expressed a desire to increase the complexity of models by adding more physics, increase the size of models, and decrease the turnover time to complete the growing number of runs required to test all desired conditions. Interest in running models on the cloud rather than on owned hardware was also expressed. The meeting provided a good opportunity to remind users that PHOENICS provides the CFD power underlying the WindSim Software. CHAM's presentation was designed to give the audience a sense of the interesting, useful and complex features being worked on here, and to underline that PHOENICS is integral to driving much of the progress they seek.

Contact Us

Should you require any further information on any of our offered products or services, please give us a call on +44 (20) 8947 7651. Alternatively, you can email us on sales@CHAM.co.uk

Our website can be viewed at www.CHAM.co.uk and we are on the following social me