PHOENICS News

PHOENICS – Empowering Engineers Spring 2018

"We have utilised CHAM software for datacentre projects and have found it easy and versatile to use. Following their training course CHAM gave very helpful technical support especially in our building services application."

Chris Lee, Johnathan Hart Associates

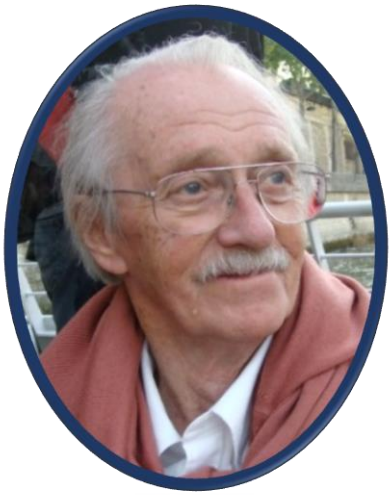
This Edition:

News from the world of Computational Fluid Dynamics: PHOENICS News designed by Robynne Moynihan

Celebration of the Life and Achievements of Professor Brian Spalding FRS FREng

Friday April 20 2018

Venue: Room 300, CAGB, Imperial College London, Exhibition Road, SW7 2AZ



Colleagues and Friends are invited to join a celebration of the life and achievements of Brian Spalding. The day will comprise a series of short presentations covering Brian's life as an Engineer, Scientist, Person, Poet and Lover of life as per the programme below.

Programme

10:00	Registration and Coffee
10:30	Welcome
10:45	Andrew Pollard - Brian Spalding – the Early Years
11:00	Brian Launder - Recollections of a Junior Lecturer with DBS
11:15	Marcel Escudier - Memories of DBS and Others
11:30	Jim McGuirk - Remembering DBS as Teacher and PhD Supervisor
11:45	Derek Bradley - Brian Spalding and Combustion Lift-off
12:00	Alan Swanson - Brian Spalding as a Trade Union Leader
12:15	Norberto Fueyo - Few Painters Invent New Colours: Brian Spalding and Turbulent Combustion Modelling
12:30	Lunch
14:00	Steven Beale - Brian Spalding: A Latter-Day Students' View
14:15	Sergey Sapozhnikov - The Poetry of Brian Spalding: A Video
14:30	Said Elghobashi: The Telegram that Changed my Life
14:45	David Gosman: Brian Spalding and the Origins of Commercial CFD
15:00	Suhas Patankar: Brian Spalding's Profound Impact on CFD
15:15	Memories of Brian at CHAM: John Ludwig and Mike Malin
15:30	Tea
15:45	Wolfgang Rodi: Brian Spalding and ERCOFTAC
16:00	Kemal Hanjalic: Brian Spalding and ICHMT
16:15	Jana Levich or Deputy: The Levich Affair
16:30	Milana Zaric: Video
16:45	Colleen Spalding - Life with Brian

Following the meeting there will be a dinner at the Ognisko Restaurant, 55 Exhibition Road from 1900. The cost for the meal will be £50 per person and partners are most welcome.

Development of the Stream Recognition Model of Transported Probabilities of Turbulent Flames:

By S.V. Zhubrin | Independent Researcher | December 2017 |svzhubrin@yahoo.co.uk

Introduction:

It is well known that the turbulent mixing of fuel and air to form industrial flames is dominated by turbulence-chemistry interactions. The purpose of this study is to provide combustion engineers with a reasonably simple, computationally economical, yet realistic and comprehensive way of predicting the mean and fluctuating structure of industrial turbulent flames. Consequently a relatively simple engineering method known as the Stream Recognition Model (SRM) is developed to calculate estimates for the probabilistic properties of turbulent combustion. The method is based on the Multi-Fluid Model (MFM) concept of Professor Brian Spalding [1] and the Multi-Environment Method (MEM) of Professor Rodney Fox [2]. The MEM has been termed the multi-peak presumed-PDF mixing model by Professor Bjorn Hjertager [3], and this worker has applied it to predict the inert turbulent mixing in the wake of two streams of differing composition.

The SRM, has been developed and implemented by the present author in PHOENICS, by using its powerful In-Form facilities for user-generated physical models. It combines the MFM and MSM approaches in such a way that use is made of the advantages of its predecessors, but with little inheritance of their drawbacks. SRM constitutes a transported-probability approach to combustion which requires a coarser discretization of variable space than the MFM, and it involves a more accurate treatment of probability fluxes than both the MEM and the MFM. The main advantage of SRM is that it can preserve the efficiency and accuracy of CFD calculations of fluctuating properties within reasonable computer time. The detailed technical description of the SRM and its applications are now publicly available online [4, 5], but some extracts are provided below to exemplify

Model Concept:

The central idea behind SRM is that a combusting flow is assumed to comprise a homogeneous blend of three streams sharing the same set of flow velocities, as well as mixture density and specific heat, namely that of the fuel gas (1), the oxidant (2), and the producer stream (3). The first two streams usually act as donors providing the third, in a probabilistic manner, with reactants to produce combustion products by thermo-chemical transformations. The latter are assumed to take place mainly within the producer-acceptor stream.

Conservation Equations:

Mathematically, SRM is based on the set of Eulerian conservation and transport equations to provide probabilistic tracking of three streams. The local probabilities of each stream are obtained from a special type of transport equation. The latter are of the standard form for general conservation, but with source terms arising from probability fluxes transferred from reactant streams into a producer one.

The sources created by the probability fluxes comprise inter-stream turbulence-probability interactions. Two kinds of such interaction are considered; namely, a direct mass transfer from (1) and (2) to (3), and also mass transfer to (3) resulting from the collision of two other streams. Such a representation provides the truly indiscriminate interactions between streams, in contrast with MEM's direct-mechanism only, and MFM's solely collision-driven *modus operandi*.

The additional conservation equations of the SRM are used to calculate in-stream attributes, such as enthalpy, temperature, element and species mass fractions, etc. The stream-weighted, mean and fluctuating characteristics are then readily computed. The details of the complete set of transport equations, as well as auxiliary and additional calculations can be found elsewhere [4, 5], together with the computational algorithm used to compute the transported stream probabilities, flow field, and stream-attribute calculations. The complete SRM was implemented into PHOENICS by using its powerful In-Form facility for user-generated physical models.

Applications:

Elsewhere [4,5] the SRM has been validated against experimental data and where appropriate, comparisons have been made with Simple-Chemical-Reacting-System (SCRS), Eddy-Dissipation Model (EDM) and MFM simulations. In these studies detailed results were reported in terms of plots of stream probability distribution, temperature, mass-fraction contours and distributions of their fluctuations and related correlations, fuel and air utilisation, pollution indices, and also flow-field velocity vectors. A very small selection of the results are reproduced below in terms of comparisons with measured data.

Figure 1 compares the measured and predicted distribution of the normalised root-mean-square concentration fluctuations along the axis of a cylindrical chamber containing isothermal coaxial jets of different composition. The Craya-Curtet number for this inert coaxial-jet system is 0.875, and it can be seen that there is good agreement between the SRM predictions and the measurements reported in [6]. The Craya-Curtet number provides a dimensionless measure of the ratio of momentum flux of the co-flowing stream to that of the central jet.

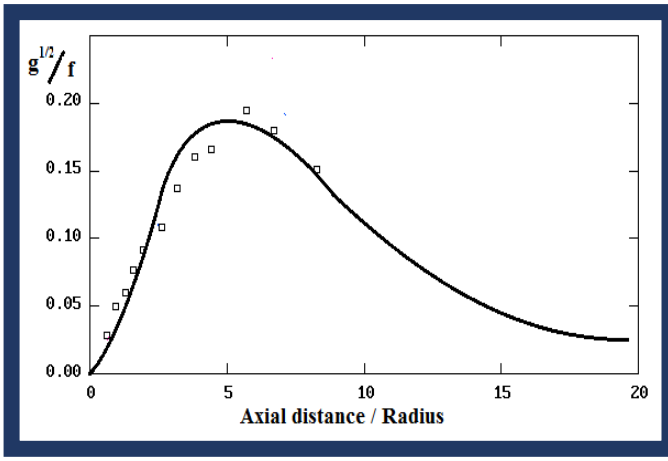


Figure 1: Time mean value of centre-line concentration fluctuations in coaxial jets Lines -SRM predictions [4], Symbols-experiment [6].

For a turbulent diffusion flame produced by a central, carbon-monoxide circular fuel jet reacting with a coaxial annular air stream, Figure 2 compares measured and predicted distributions of mean temperature along the axis of the combustion system. This case was studied experimentally by Razdan and Stevens [7].

Figure 2 shows that there are significant differences between the SCRS (Simple-Chemical-Reacting System) results, which assumes infinite-rate chemistry, and the experimental data. The SCRS model fails to fit the data reasonably well, both in terms of location and magnitude of the maximum temperature. In contrast, the results produced by both the MFM and SRM are in acceptable agreement with the measurements.

In [5] the SRM was extended to simulate a turbulent premixed flame with finite-rate chemistry effects in both relatively fast and slow modes. These combustion processes were simulated in a geometrically idealized, but operationally typical gas-turbine combustor. The mean and fluctuating characteristics of combusting flow, and also their correlations were calculated together with nitric-oxide emissions. This work was largely of a qualitative nature to demonstrate capability, and so result extracts are not reproduced here.

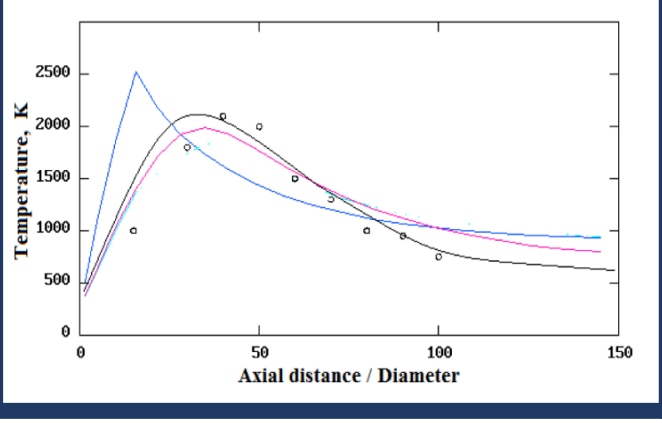


Figure 2: Time mean value of centre-line temperature in a turbulent diffusion flame Line - SRM [4] Blue line – SCRS, Red line- MFM, Symbols, -experiment [7].

Concluding Remarks:

The SRM probabilistic flow-chemistry module has been implemented in PHOENICS by the author using In-Form, and the present study has demonstrated the capabilities of this novel approach for modelling turbulent-combustion processes. The method can handle combusting flow involving fast, finite- and low-reaction rates, and is quite broad in its capabilities. In particular, it is readily applicable to both premixed and diffusion flame computations.

The procedure has been applied successfully to a number of laboratory case studies, and those of realistic three-dimensional geometry and operating conditions. These applications have demonstrated that it is possible to calculate fluctuating *in-stream, stream-weighted* and *mean* flow properties, as well as probabilistic turbulence-chemistry interactions; and to assess details of the thermal and polluting performance of a combustion unit - all achieved simultaneously and with relative ease.

The existing, earlier models [1, 2] of transported probabilities have been combined, and perhaps, the simplest kind of model that permits predictions of both magnitudes and probabilities of fluctuating properties has been developed. It accounts successfully for most practically important features of turbulence-chemistry interactions, and as we have seen here, its use has led to satisfactory predictions of mixing in inert turbulent flows as well as those of a reacting kind.

The field distributions of stream probabilities generated by SRM provide valuable insight into the fluctuating nature of combusting flow. Computations of fluctuating properties and their correlations, which are inexpensively derived from present approach allow the intermittency factors to be calculated through the probabilities of different streams present in a flow system.

There is, of course, substantial scope for further model development and improvement. For example, a larger number of participating streams could be accounted for by using more general stream-interaction mechanisms. The boundary heating effect (at the internal and external walls) needs to be represented as a separate addition to the stream enthalpies. The inclusion of a radiation model to handle turbulence-radiation interactions should perhaps, be given preferential consideration.

The assumption of the homogeneous nature of stream mixture can also be relaxed by allowing different streams or groups of them to move with their own velocities.

All of these developments would be a natural extension to the work described in this article, and it is fairly straightforward to extend the present theory in these directions. Yet it is maintained that the achieved level of agreement between predictions and measurements is satisfactory, and the model is already sufficiently developed to justify its use for many engineering purposes.

References:

1. D.B.Spalding, Models of turbulent combustion, in: Proceedings of the Second Colloquium on Process Simulation, Helsinki University of Technology, Espoo, Finland, 1995, pp. 719-730

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Multi-Scale Modelling of Thermo-Chemical Performance of Ammonia Cracking Unit V. Agranat, S. Zhubrin | Applied Computational Fluid Dynamics Analysis (ACFDA), Canada |info@acfda.org | V. Erenburg, G. Finkelshtain, E. Gamerman and M. Lerner | GenCell Ltd., Israel | team@gencellenergy.com

Ammonia Cracking Units (ACUs) play essential roles in mobile applications of fuel-cell technologies such as auxiliary electricity generating devices. Mathematical modelling of a practical ACU requires the coupling of geometric and fluid-mechanical aspects with chemical-kinetics complexity at unit and at system - scale levels simultaneously.

The catalytic cracking of ammonia depends upon gas-phase and heterogeneous reaction mechanisms that can involve a number of chemical reactions. Direct chemistry coupling at different levels requires the significant extensions of the built-in capabilities of general-purpose Computational Fluid Dynamics (CFD) codes. The latter should handle, in-parallel or simultaneously, the geometry of cracking units, peripheral devices, such as heat exchangers and their assembly configurations in a way similar to one shown in previous developments [1-3].

The present paper describes a novel capability to couple the full chemical kinetics with CFD and system-level analysis on the basis of the general-purpose CFD software, PHOENICS (http://www.cham.co.uk/phoenics.php). The approach exploits the structure of cracking units, in which the combined gas-phase and catalytic heterogeneous chemistry is confined within geometrically simple channels, and the engineering models of peripheral units.

Gas flow and catalytic combustion over the internal surfaces of the reaction zone walls are used to achieve thermal control. Hot combustion products from a fuel-cell purge/tail-gas exothermal oxidation taking place in a combustion zone are used to support the endothermic ammonia cracking in the reaction zone. Figure 1 illustrates a typical configuration of such a unit.

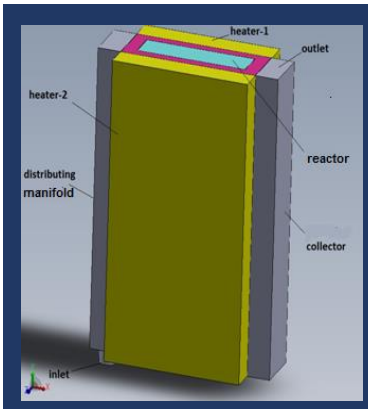

Figure 1. Illustration of ammonia cracking unit

Process and unit coupling is accomplished with the user-defined settings of the In-Form capability available in PHOENICS (http://www.cham.co.uk/phoenics/d_polis/d_enc/in-form.htm). Fluid flow and heat- and mass transfer within the reaction and combustion zones are represented by CFD models that are developed to accommodate the appropriate chemical transformations. Coupling is made via the exchange of convective-radiation heat fluxes at the walls between zones. In addition to internal fluid flow, the customized PHOENICS model also represents immersed-solid heat transfer within the reactor walls and heat- and mass exchange with the external environment and auxiliary equipment.

Figure 2 illustrates a coupled solution for a particular ACU. The modelling results show the air oxidant path lines that are coloured by particle variables. The path lines display a relatively complicated three-dimensional flow pattern. The hot products of purge-gas oxidation are cooled by heat transfer to the reaction zone in support of the endothermic reforming of ammonia. Heat transfer to the outer reactor walls also cools the combustion product flow.

A powerful CFD simulation capability couples complex gas - mixture flow and heat- and mass transfer with highly nonlinear ammonia cracking and catalytic purge-gas combustion chemistry. Such a modelling tool plays by itself an important role in providing practical solutions of the unit/system design problems of ammonia cracking technologies. The development of a CFD model for each equipment unit of an entirely coupled ammonia cracking system presents significant challenges. The creation of the computational models including mesh generation may take a long time and the total number of

computational cells required may make the calculation impractical, (i.e. the computations, if they can be done at all, may prove very time-consuming and not suitable for design-time and run-time predictions.

Therefore, a computational interface has been developed, within the main computational loop of the CFD solver, for the thermo-chemical coupling links, which allow the system and heat - exchanger network model of low scale to co-simulate with the higher-scale CFD simulations. By co-simulating a system model with CFD, the more realistic boundary conditions and component models are obtained economically, providing a deeper understanding of complex links in ammonia cracking systems.

A typical multi-scale modelling procedure uses ACUTE (Ammonia Cracking Unit's Thermo-Chemical Equations), a specifically developed PHOENICS-based system-level module, to model the entire assembly of ammonia cracking system including ACU and a network of supporting heat exchangers. The ACU itself can be modelled in detail using either fast-track lumped or more complex CFD technique (ACU2D or ACU3D), with the co-simulation to ensure that a two-way, bilateral exchange of inlet/outlet parameters between the ACUTE and CFD models provides a continuity of mass, heat and momentum transfers.

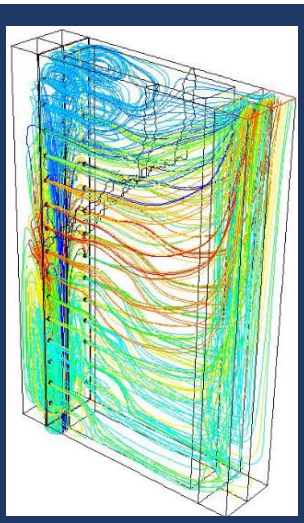

Figure 2. Path-lines in combustion zone coloured by particle variables

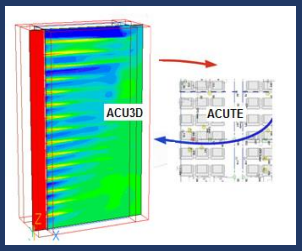

Figure 3. Coupled application of ACU3D and ACUTE models

Initially the co-simulation module attempts to procure a converged solution with the ACU3D/ACU2D model. Resultant boundary conditions and/or flow rates are exchanged, as shown in Fig. 3, with the system-level ACUTE model so that it may update its solution, exchange and update the boundary conditions for the ACU3D/ACU2D model. There are two 'controls' that the user may use to influence overall convergence behaviour. These are the number of iterations of the ACU CFD solver before a data exchange of boundary conditions, and a relaxation factor which controls the extent of changes between successive calls to the ACUTE solver. When these parameters are appropriately specified, a converging iterative behaviour is generally obtained.

This paper provides an overview of the model that is under development by GenCell Ltd. in collaboration with ACFDA for computer predictions of the technological behaviour of ammonia cracking units. This is a system-level model with a co-simulation using CFD techniques considering the thermo-chemical performance of all components that exchange mass and energy to produce the fuel-cell-generator device's thermal and electrical output.

The models summarized in this paper are currently in use by GenCell. They indicate the correct performance trends and already have helped to explain a number of important observations both qualitatively and quantitatively. It is expected that testing and analysis of current implementations will lead to model refinements and enhancements. Furthermore, GenCell is carrying out a program of experimental work that will result in a set of comparative tests. Those will be used to further validate, calibrate and improve the models. Subsequent papers will report model details, enhancement and validation efforts, as well as the simulation and observation results obtained, and technological effects achieved.

References:

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New Free Surface features in PHOENICS

By Jalil Ouazzani, ArcoFluid (Bordeaux, France) & ArcoFluid Consulting LLC (Orlando, USA) – jalil@arcofluidconsulting.com

1. The THINC – WLIC Method:

high-resolution interface-capturing schemes for immiscible-fluid and free-surface flows, as well as a facility for modelling surface-tension effects at the interface. This article reports on further free-surface developments for use in PHOENICS 2018 Version 2, which is scheduled for release later this year. This upgrade will include the THIN/WLIC [2-3] interface-capturing scheme, and an enhanced surface-tension model that accounts for the contact angle between the interface and solid walls, as well as the dependence of surface tension on temperature.

The hyperbolic tangent function is used to devise a conservative, oscillation- and smear-free scheme called the THINC (tangent of hyperbola for interface capturing) scheme. This scheme shows competitive accuracy compared to most existing methods without geometrical reconstruction. The WLIC (weighted line interface calculation) method extends the THINC scheme to multi-dimensions by taking the average of line interfaces along each coordinate direction with weights calculated from the surface normal [3].

The hyperbolic tangent is the simplest continuous function which itself has the step-jump distribution property. The THINC scheme uses the piecewise modified hyperbolic tangent function:

$$F_i(x) = \frac{\alpha}{2}\left(1 + \gamma tanh\left(\beta\left(\frac{x - x_{i-(1/2)}}{\Delta x_i} - \tilde{x}_i\right)\right)\right).$$

The parameters α, β, γ are important for determining the quality of the numerical solution.

The original THINC-WLIC method is fully explicit, but the SIMPLEST algorithm of PHOENICS does allow the use of an implicit method and the conservative form of the marker variable, if so desired.

The THINC-WLIC method was tested on a classical benchmark for free surface flows, namely the Rider-Khote [4] reverse vortex where the velocity is time and space dependent. A circle of radius 0.15 is initially centred at (0.5, 0, 75), and then transported by the THINC/SW (slope weighing [2]) scheme from 0 to T/2 clockwise, and from T/2 up to T=8 anticlockwise. The numerical results at T/2, T and other intermediate times are presented in Figure 1 below. The interface has been deformed into a spiral at T/2 and is well resolved except that the thin tail is broken into small droplets in a way quite like all other existing VOF schemes.

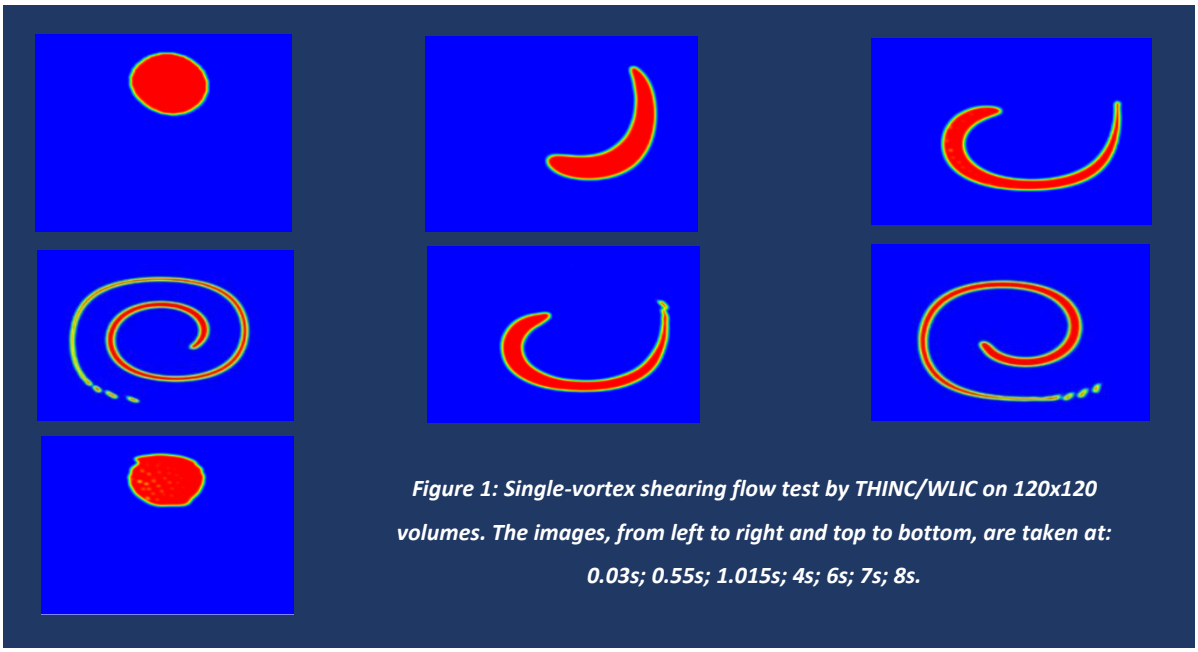

Figure 1: Single-vortex shearing flow test by THINC/WLIC on 120x120 volumes. The images, from left to right and top to bottom, are taken at: 0.03s; 0.55s; 1.015s; 4s; 6s; 7s; 8s.

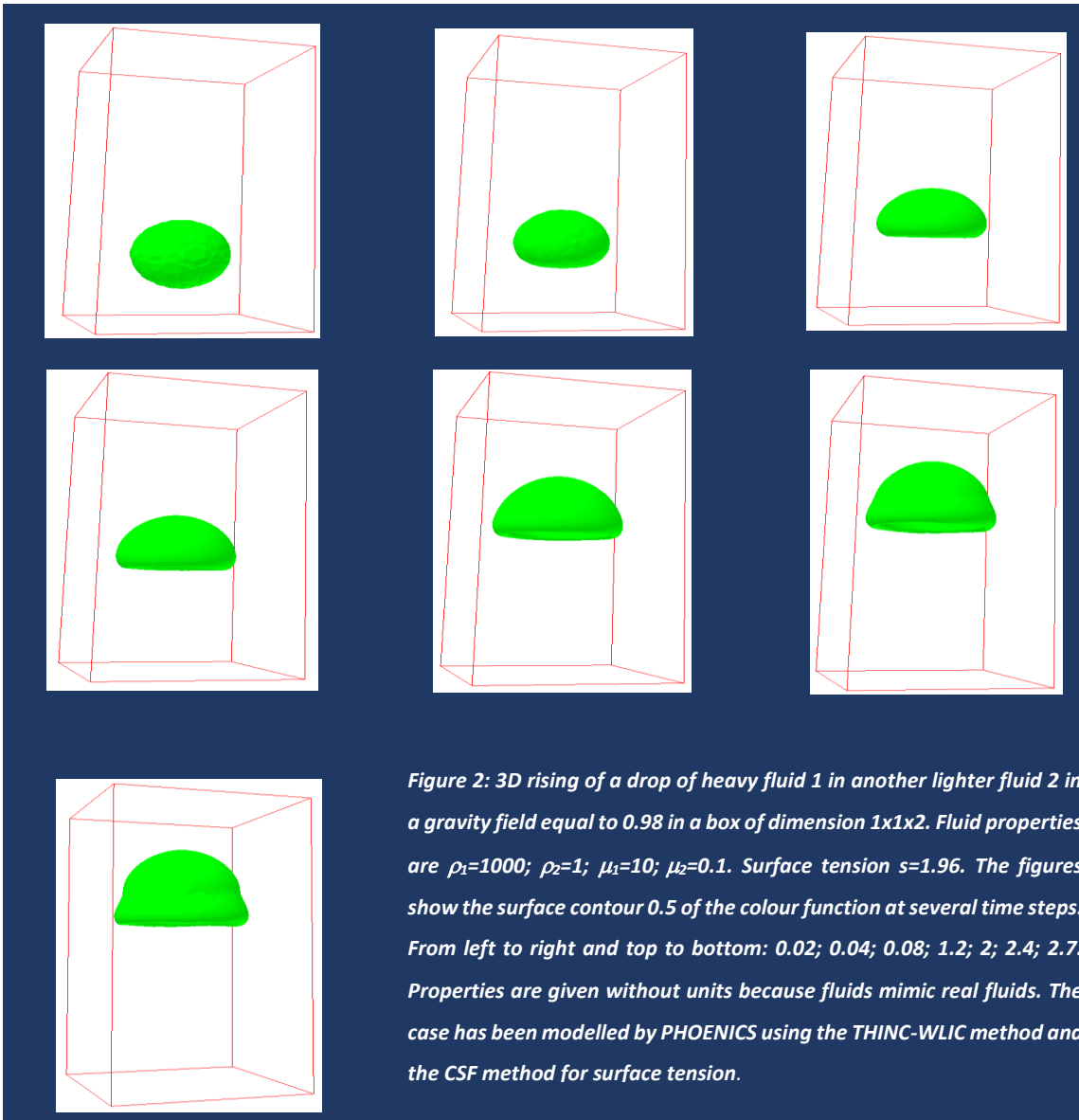

Figure 2: 3D rising of a drop of heavy fluid 1 in another lighter fluid 2 in a gravity field equal to 0.98 in a box of dimension 1x1x2. Fluid properties are ρ_1=1000; ρ_2=1; μ_1=10; μ_2=0.1. Surface tension s=1.96. The figures show the surface contour 0.5 of the colour function at several time steps: From left to right and top to bottom: 0.02; 0.04; 0.08; 1.2; 2; 2.4; 2.7. Properties are given without units because fluids mimic real fluids. The case has been modelled by PHOENICS using the THINC-WLIC method and the CSF method for surface tension.

2. The surface tension model: Capillary and Marangoni terms:

Surface-tension effects are represented in PHOENICS by the continuum-surface-force (CSF) model of Brackbill [5]. This model only acts near the interface, as defined by the transition region for the marker variable ϕ, and the continuous volumetric force is calculated from:

$$F_\sigma = \int_S \sigma\kappa\delta(x - x')dS = \sigma\kappa\nabla\phi$$

where ϕ is the volume fraction, $\mathbf{x}$ the position, $\mathbf{x}'$ the interface, σ is the constant surface-tension coefficient, and κ the curvature of interface given by $\kappa = -\nabla \cdot \left(\frac{\nabla\phi}{|\nabla\phi|}\right)$. The gradient $\nabla\phi$ is evaluated directly from the two values straddling the interface. For constant σ, the surface-tension force can be expressed by:

$$F_\sigma = \sigma\kappa\nabla\phi = -\sigma\left(\nabla \cdot \left(\frac{\nabla\phi}{|\nabla\phi|}\right)\right)\nabla\phi$$

The free surface mean curvature κ is defined by:

$$\kappa = \frac{1}{|\vec{h}|}\left[\left(\frac{\vec{h}}{|\vec{h}|}\cdot\nabla\right)|\vec{h}| - (\nabla\cdot\vec{h})\right]$$

where $\vec{n} = \nabla\Phi$ is the normal. This formulation enables better accuracy when using finite differencing to compute gradients, but when a more accurate method is used to compute the normal, such as the Height Function [6-7] or CLSVOF (combined level-set VOF) [8], one can compute $\kappa = \nabla\cdot\frac{n}{|n|}$ directly. These approaches have been implemented as options in PHOENICS, but they are not as accurate as using finite differences to compute the normal. Another option introduced in PHOENICS is to compute $\kappa = \frac{1}{|\vec{n}|}[(\boldsymbol{n}.\nabla)\log(|\vec{n}|) - \nabla\cdot\vec{n}]$. There is a need to evaluate and compare these different approaches for various test cases and applications.

If surface tension is variable and depends on temperature and/or concentration (the so-called Marangoni effect), then the surface tension force has an extra term in the momentum equation, namely:

$$F_\sigma = \sigma\kappa\vec{n} + \nabla_s\sigma$$

where the surface gradient is formulated as follows:

$$\nabla_s = (I - \vec{n}\vec{n})\cdot\nabla$$

The notation $\vec{n}\vec{n}$ is used for the outer product of vectors, i.e. $\vec{n}\vec{n} = \vec{n}\vec{n}^T$. The terms on the right-hand side of the above equation for F_σ can be identified as the capillary and Marangoni forces, respectively [9].

The following two-dimensional example considers the thermocapillary migration of three water droplets within an air-filled cavity under zero-gravity conditions. PHOENICS is used to predict how the droplets migrate in a varying temperature field due to the thermal Marangoni effect. The fluids are initially at rest, the surface tension varies linearly with temperature, and the initial temperature field varies linearly, with the bottom and top surfaces of the cavity maintained at 20°C and 50°C, respectively. The migration of the droplets is driven by temperature gradients, which bring about a surface-tension gradient driving the flow from the cold to the hot region.

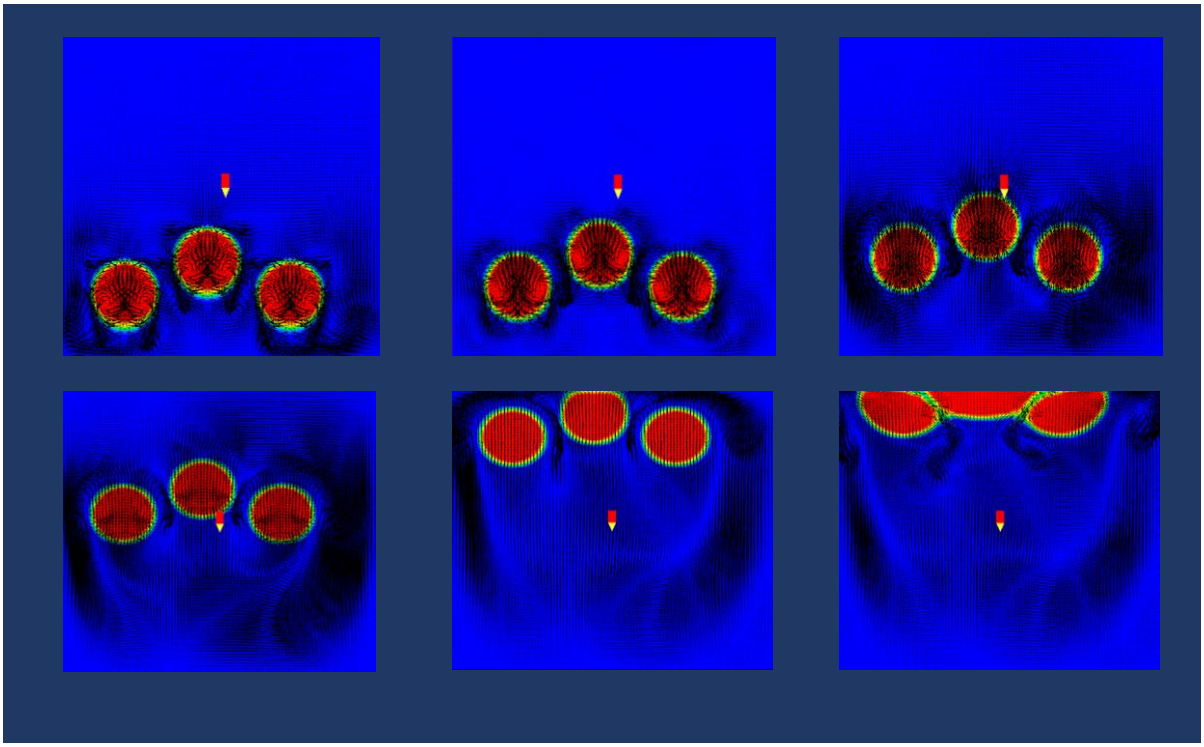

Figure 3: After a short time, rolls start to form inside the droplets and motion is triggered by the varying surface tension. Droplets are migrating from the cold (bottom) to the hotter region (Top). The figures show color function and velocity vectors at different instants.

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News from CHAM Agents:
Champion – Photographs of a PHOENICS seminar in BIM
Jasmine Li

PHOENICS Development Road Map – 2018:

General:

The current release version of PHOENICS (PHOENICS 2018 v1.0 (dated January 2018) is described at:
www.cham.co.uk/phoenics/d_polis/d_docs/tr006/tr006.pdf

PHOENICS-2018- v2.0 – Summer 2018:

The next PHOENICS-2018 release becomes available mid-2018. Major items included within this version are:

- Auto wall functions for k- ω based models
- Thermo-phoresis for the Drift Flux Model (DFM)
- Full treatment of inclined surfaces for DFM
- Inclusion of VOF – THINC
- Inclusion of Marangoni effect and contact angle for all free-surface models.
- Acceleration of parallel solver using HYPRE solver
- IPSA model improvements for modelling dense solid media (e.g. blast furnace, avalanche)
- Inclusion of Belgian / Dutch / FRS fire models (FLAIR)
- Cavitation model
- Shallow water model made accessible through GUI
- Heat and scalar source at surfaces of facetted objects.
- Bug fixes and small enhancements to Core and FLAIR,

PHOENICS-2018- v3.0 – Autumn 2018:

Items in-progress for inclusion in next release of PHOENICS-2018

- Inclusion of replacement multi-grid and coupled solvers
- Re-evaluation of Unstructured PHOENICS
- Continued improvement of FGV
- PARSOL (X-PARSOL) revision
- Curved 'thin plate' object.
- Flow-induced movement of blockages