What's New in PHOENICS-2023

CHAM

Experts in CFD Software and Consultancy

PHOENICS-2023

If it flows - PHOENICS models it

PHOENICS models flow. It is used for CFD applications including environmental and, engineering, and has been for over four decades. Colleagues who worked with Brian Spalding to create PHOENICS use their extensive CFD expertise and experience to keep it updated and relevant.

PHOENICS simulates, tests, improves, and optimizes, product performance without the cost of real-time tests. The code's reliable and extensive physics create models needed for all fluid-flow applications or, if preferred, our skilled technical team will undertake the work for, or in conjunction with, clients.

See inside to get an idea of new features, changes, updates and bug fixes in PHOENICS-2023; and of work in progress.

PHOENICS-2023 will be available to current Users who update under annual maintenance agreements. New PHOENICS Users will receive this version automatically.

Colleen Spalding
Managing Director

PHOENICS-2023 Features

1) *UnStructured PHOENICS (USP) Revision*
2) *Volume of Fluid (VOF) to include Steady State*
3) *Wind Object includes Pasquill Stability Conditions*
4) *Ergun Pressure Drop for BLOCKAGE*
5) *Thermal Heat Capacity for Non-Participating Blockages*
6) *EARTH Convergence Monitor includes Change Saving Facility*
7) *Log-scale Contours in Viewer*
8) *Plot VTK Files in Viewer*
9) *Disable File Numbering for Intermediate Dumps*
10) *Bug Fixes*
11) *Work In Progress:*

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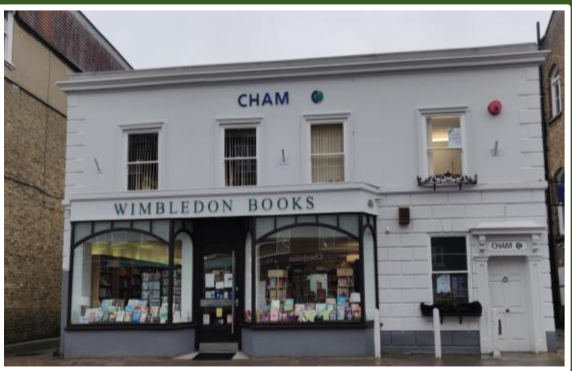


1) UnStructured PHOENICS (USP)

PHOENICS does not always need a structured grid. Using unstructured PHOENICS is computationally economic. Grid cells in the unstructured version remain predominantly six-sided and, except where obliquely cut by surfaces of physical objects, of cartesian or cylindrical-polar shape. The faces may have unequal cell numbers on opposite sides; usually one on one side and two/four on the other.

In effect, different grids are used for different variables so, if solids and fluids are in the same domain, cells in the solid part are used only for temperature as no pressures, velocities, or other scalars, are computed there.

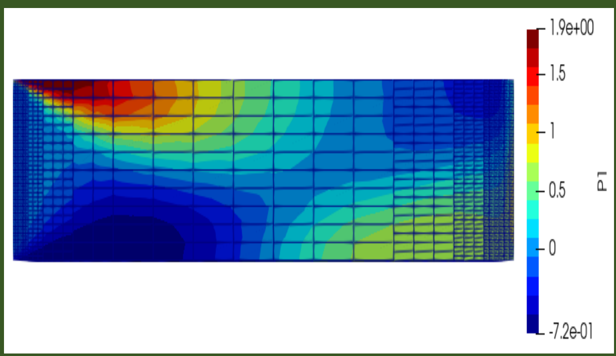
UnStructured and structured PHOENICS exist simultaneously in one executable and have much in common.

Points of similarity include:

- Problem-set-up data are supplied via a q1 file to Satellite and via an eardat file to EARTH;
- Calculation outputs appear in RESULT / PHI files;
- Graphical output to monitors appears similar.

Points of difference include:

- USP requiring additional instructions from users regarding the grid to be used.
- Data formats written to RESULT / PHI files differ.



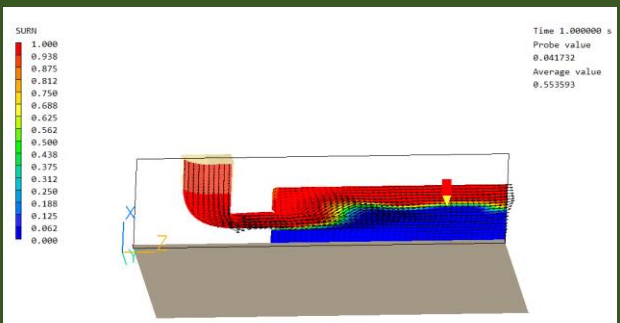
UnStructured PHOENICS-2023 will include:

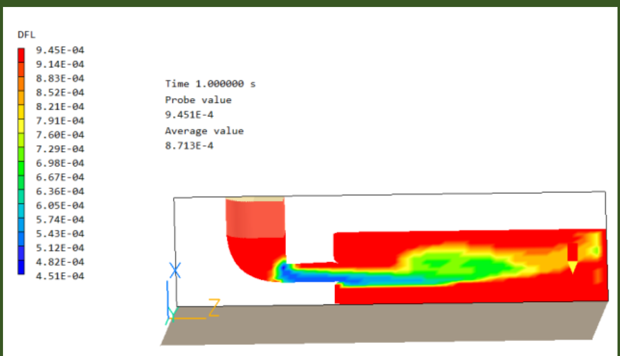
- USP mesh display in VRE;
- USP solutions in VRV
- Allowance for parallel operation;
- Physical property formulae used in PROPS file;
- FLAIR Comfort Indices;
- Heat source on outside of 198 blockages
- Compressible / high speed flow
- Fire object
- Wind object

Compressible flow in USP works for both low- and high-speed flow with divided grids.

2) Volume of Fluid (VOF)

Having a steady-state extension to VOF allows certain classes of free-surface flows to be solved steady-state as opposed to the current requirement that all VOF cases are run transient. This should reduce computer time drastically for such steady state flows.





3) Wind-Object Upgrade

PHOENICS and PHOENICS-FLAIR are used extensively to model the atmospheric boundary layer (ABL) in wind-engineering applications, such as pollutant dispersion, urban wind-comfort studies, and optimization of wind-farm placement. For such studies, wind inlet profiles and boundary conditions can be specified automatically via the WIND object in PHOENICS.

The Wind Object has been upgraded to include Pasquill Stability conditions which allows external wind calculations with stratified boundary layers to be performed. This applies to density-differences due to temperature or concentration changes – as in a release of dense gas.

These Pasquill-stability classes define 6 atmospheric-stability classes labelled A to F based on wind speed, sun insolation and cloud cover.

Wind speed (m/s)	Daytime Insolation			Night time conditions	
	Strong	Moderate	Slight	Thin overcast >= 4/8 low cloud	<=3/8 cloud
< 2	A	A-B	B	-	F
2-3	A-B	B	C	E	E
3-5	B	B-C	C	D	D
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

Table 1: Pasquill Stability Classes: A (very unstable), B (moderately unstable), C (slightly unstable), D (neutral), E (slightly stable), F (moderately stable)

For unstable classes, increased vertical mixing occurs as ground solar heating increases near-surface air temperature, and decreases density. Neutral class D occurs early morning/evening when solar heating is negligible and wind speed dominates vertical mixing.

For stable classes, solar heating is less than ground cooling; this usually occurs at night. Near-surface air density is increased so that vertical mixing is suppressed. In modelling hazardous-gas dispersion, stable conditions are used to represent worst-case scenarios due to reduced mixing and dilution of said gas into the atmosphere. Class F defines a standard weather condition used to model dispersion of toxic substances for land-planning in the UK and elsewhere.

Implementation in PHOENICS is generic in terms of gravitational and wind directions, and covers Pasquill stability classes A to F by using the Monin-Obukhov Similarity Theory (MOST) to specify boundary conditions.

In this release account is not taken of MOST in turbulence transport equations and wall functions, and the energy equation is not solved in terms of potential temperature.

The required Pasquill Stability class can be selected directly from the WIND object dialog:

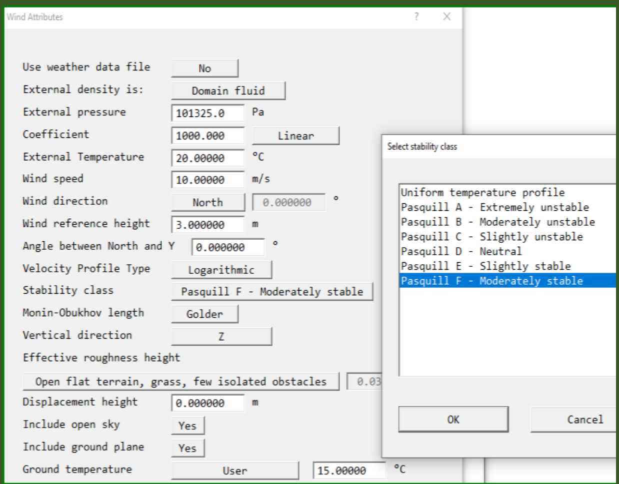
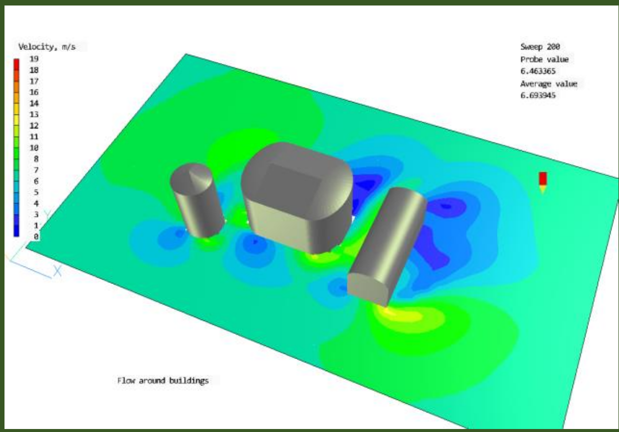


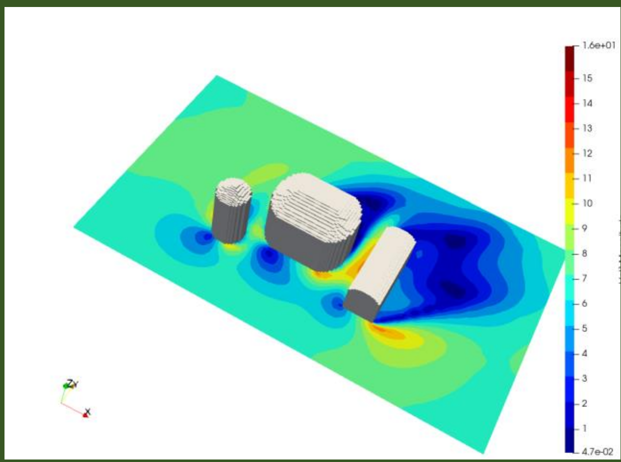
Figure 1 Selecting the Stability Class

Part of the USP upgrade has been to enable the WIND object to handle uneven terrains which could always be done in Structured PHOENICS.

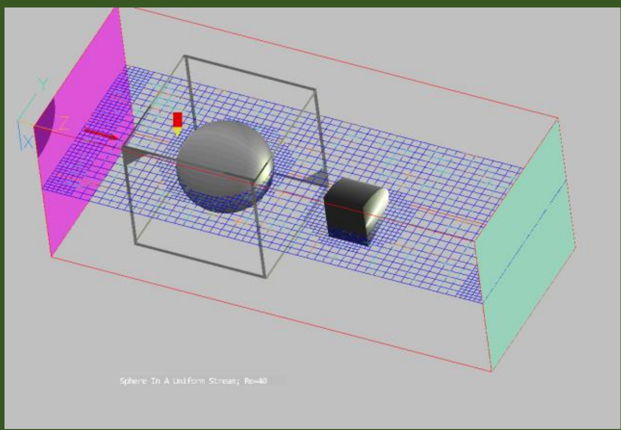
Wind object using a structured grid:



Wind Object in USP:



USP Grid refined near buildings:



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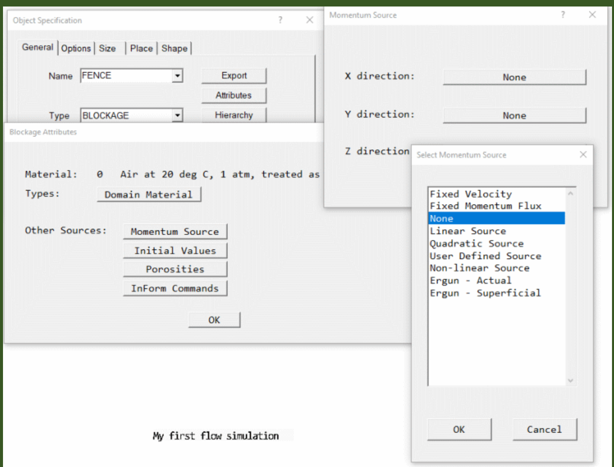
4) Ergun Pressure Drop for BLOCKAGE

The list of Momentum Sources that can be applied by a fluid BLOCKAGE object has been extended to include the Ergun formulation:



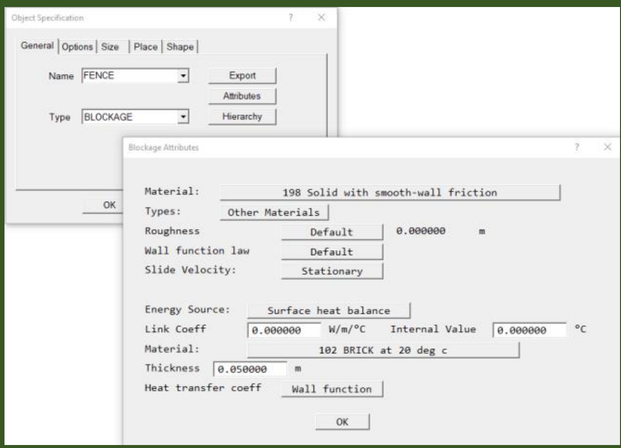
The force is:

F = mass-in-cell* $(150*v*(1-P)^2/(P^3*D_p^2)*(V-Vel_p) + 1.75*(1-P)/(D_p*P^3)*V_{abs}*(V-Vel_p))$ where:

- v is laminar kinematic viscosity,
- P is gas porosity (1=open, 0 = blocked)
- D_p is the particle diameter
- V_{abs} is the local absolute velocity
- V is the velocity of the packed bed
- Vel_p is the local velocity, U1, V1 or W1

For 'Actual', the porosity value is applied to the cell face areas, so the velocity is the actual device velocity. For 'Superficial', the face areas are not adjusted, and the velocity is the approach velocity. The form of the source is modified to account for this. The expression above is the 'Superficial' form.

5) Thermal Heat Capacity for Non-Participating BLOCKAGE



For a non-participating BLOCKAGE (material 198), it is possible to set a heat balance boundary condition for the surface temperature.

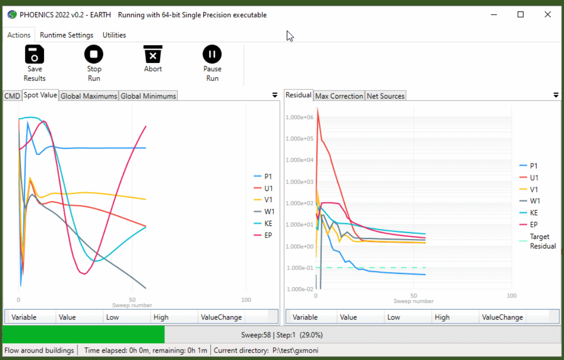
The surface temperature is deduced from a heat balance between the fluid temperature in the cell adjacent to the surface, and a user-set fictitious internal temperature.

For transient cases, the heat balance has been extended to include the thermal capacity by specifying a material and nominal thickness. The current surface temperature is stored in TWAL, and the previous time step in TWLO for plotting in the Viewer.

If the SUN object is active, the heat balance includes the solar heating.

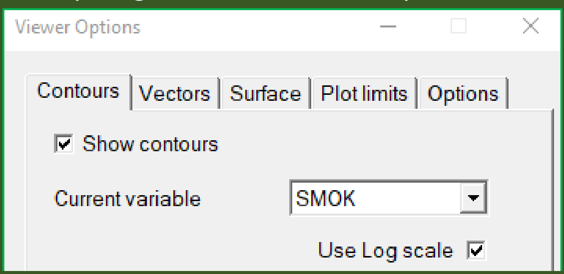
6) Earth Convergence Monitor (ECM) Update

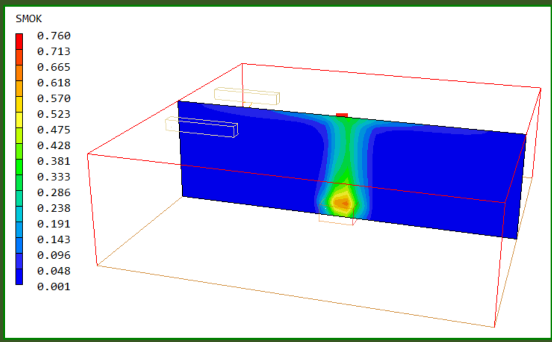
The Earth convergence monitor screen (GXMONI) was replaced in the 2022 release. The new, more modern, flexible, ECM allows any combination of available monitor graphs to be shown in a single window or on split screens in separate. It also allows various monitor windows to be positioned and sized by the User. For 2023, these changes are now saved for future use. Individual curves can be identified easily by clicking on them to highlight the selected curve. The display of numerical values in addition to the graph can be pinned for each plot.



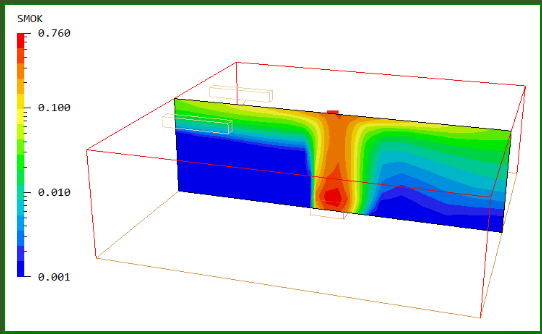
7) Log Scale Contours in Viewer

Traditionally, contour plots produced by VR-Viewer have used linear scales. In the majority of cases this is what is needed. There are occasions when, for some scalars, the range of values is so large that it becomes hard to plot sensibly in that the linear scale hides too much detail when the range of contour values spans several orders of magnitude. A typical situation might be smoke spread in a fire where, as shown, layering of smoke is masked by the linear scale.

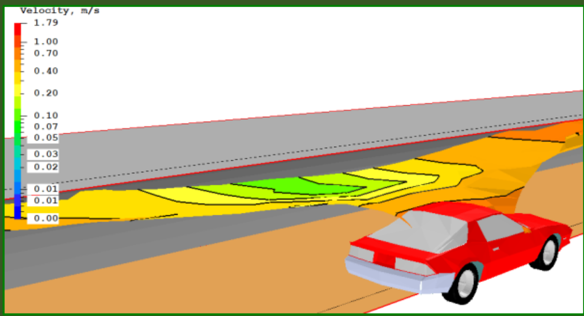


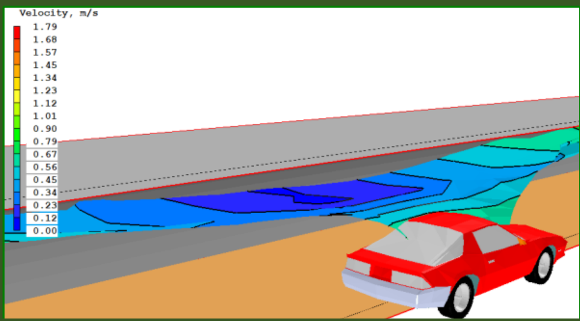


VR-Viewer now allows changing contour- to logarithmic-scale so layering becomes apparent.



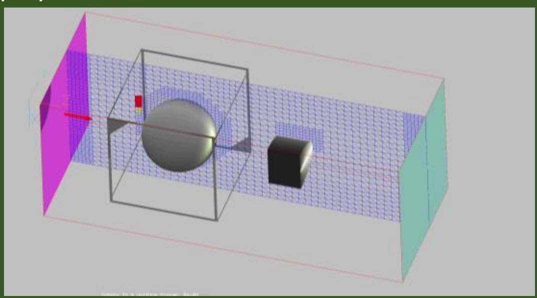
The logarithmic scales also apply to contours of a variable on an iso-surface of another. The images below show iso-surface of sight-length (SLEN) coloured by Velocity.

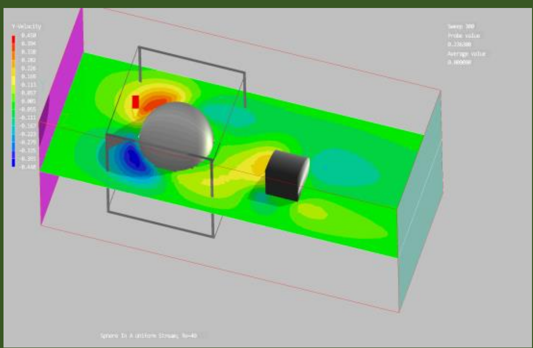


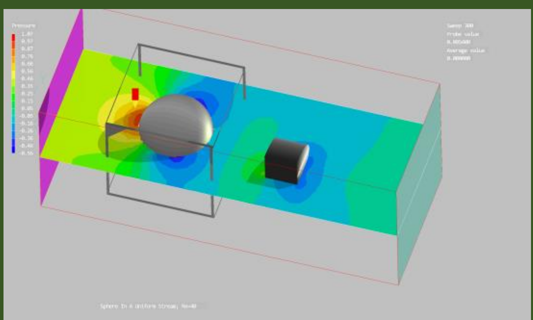


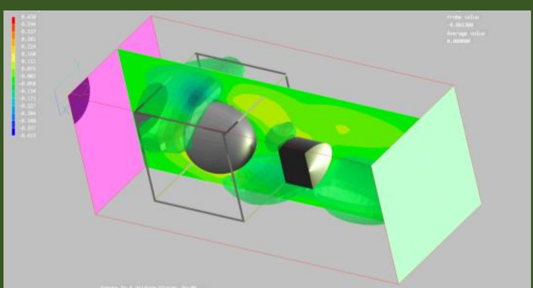
8) Plot VTK Files in Viewer

The Viewer has been extended to allow it to plot results held in VTK files. This will allow the user to plot solutions produced by Unstructured PHOENICS without recourse to third-party software. The unstructured mesh can also be displayed.







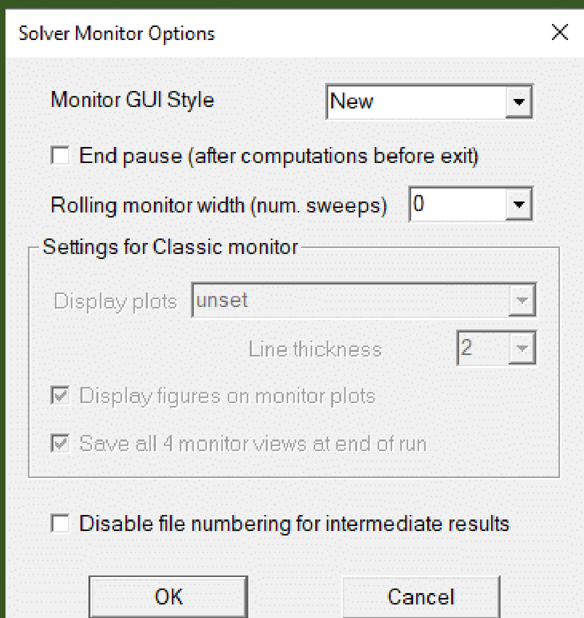


9) Disable File Numbering for Intermediate Dumps

When the Earth solver is running a long simulation, steady or transient, it is straightforward to instruct the Viewer to automatically refresh the current plot each time a new solution file is written (by right-clicking the F9 icon). This allows changes in the solution to be monitored in real time and aids in assessing convergence for steady cases - if the plot does not change from sweep to sweep, the run is converged.

For transient cases, the saved solution files can be used later to make and save animations. For steady cases the same can be done, but more often than not the saved solution files just take up disk space and are not used again.

It is now possible to switch off the saving of individual solution files for steady cases, and always just overwrite the final solution file. This preserves the ability to monitor the progress of the run in real time whilst simultaneously saving a lot of disk space.



10) Bug Fixes in PHOENICS-2023 cf PHOENICS-2022

10.1 VRE

- Improve detection of domain material name for BLOCKAGE using domain material.
- Increase internal string lengths to cope with long error messages.
- Allow for very long strings in input boxes.
- Allow for blanks in name of private solver.
- Correct menu dialog display for Bingham and Power-law fluids.

10.2 VRV

- Improve text capture when saving VBO images
- Prevent hangs caused by simultaneous incompatible operations eg starting a line plot when an animation is still running.

10.3 Earth

- Allow porous plate with pressure-drop to run in parallel.
- Allow GROUND/InForm-set specific heat to use previous sweep value to derive current sweep (eg for solidification models).
- Resolve occasional internal conflicts between TABLE object and InForm TABLE command.
- Correct error in source inflow/outflow reporting in parallel.
- Prevent occasional hang when saving files in parallel.
- Corrected ANGLED_IN/OUT not to test for surface area outside domain.
- Replace TMP1C with ENULC for ENUL=GRND7 (laminar viscosity step function of temperature).
- Correction to VOF contact angle
- Attempt to run the Drift-Flux model with no SOLVEd or STOREd aerosol variables now elicits an error message rather than causing a crash.
- Switch between 'at constant temperature (dTabs=0)' and 'over range (dTabs=1)' for CP1=GRND6 (specific heat for phase change. material); was wrong way round.

11) Work in Progress

11.1) IPSA Extension to Include Kinetic Theory of Granular Flow (KTGF)

The Inter-Phase-Slip Algorithm (IPSA) developed by Spalding allows solving full Navier-Stokes equations for each phase and has been built into PHOENICS since 1981. PHOENICS-2022 contained a new IPSA capability namely a *particle-cluster 4-zone fluidisation drag model* which is included for fluidised bed applications and characterised by four different flow regimes, namely: dense, sub-dense, sub-dilute and dilute. A blending function is introduced to provide smooth transition between the various regimes.

IPSA has been extended in PHOENICS-2023 to account for particle-particle interactions by implementing models for the solids stress tensor based on the kinetic theory of granular flow. KTGF involves solving an equation for the granular temperature, which represents the kinetic energy of the fluctuating particle velocity field. The IPSA-KTGF model, which can be operated from the GUI, facilitates the handling of important applications including dense-regime pneumatic lines, riser reactors, and fluidised-bed reactors.

11.2 Phase-Change Material (PCM) Object for FLAIR

It is proposed to implement a generalized version of the PCM model described in the Autumn 2022 Newsletter article by Peter van de Engel, of TU Delft.