Assessment of Commercial Off-the-Shelf CFD Tools Through Application to Thermal Treatment Modelling

By **Ella Schaefer, Tim Ashworth, Rob English, Sarah Swales, Ben Vickers and Euan Williamson.**

SUMMARY

- Thermal treatment to immobilise UK radioactive wastes has so far been implemented for High-Level Waste (HLW) vitrification, whereas Intermediate Level Waste (ILW) is generally encapsulated within a cement matrix. Thermal treatment offers the potential to overcome the disadvantages associated with the cementation process.
- Sellafield Ltd and Thornton Tomasetti collaborated to undertake specialised Computational Fluid Dynamics (CFD) modelling of a thermal melt pool for a Joule Heat Ceramic Melter (JHCM). This forms part of an assessment of the feasibility of deploying thermal treatment for pumpable ILW.
- The initial modelling phase, discussed here, focused on understanding capabilities and limitations of Commercial Off-The-Shelf (COTS) CFD software and different approaches for modelling particle transport. The modelling simulated the motion of gas bubbles and solid particles through a glass melt pool and assessed the sensitivity of particle behaviour to glass melt properties, particle diameter and density, for fissile materials and the reduced and noble metals that could credibly be present.
- The work demonstrated that COTS software is generally capable of modelling a simplified representation of a thermal melter with Joule heating. The analysis identified cliff-edge changes in dominant behaviour where particles would drop out of suspension, which could be used to inform and design against criticality risk.

INTRODUCTION

As of 2025, the Nuclear Decommissioning Authority (NDA) is ensuring that its operating companies undertake a full evaluation of thermal treatment use. Thermal treatment to immobilise UK radioactive wastes has so far been implemented for HLW vitrification, whereas ILW is generally encapsulated within a cement matrix.

The cementation process is well established, compatible with wet wastes and operates at low temperatures. It is notably limited by the increased volume of waste for disposal and incompatibility with some waste streams. Thermal treatment offers the potential to overcome these disadvantages.

Sellafield Ltd and Thornton Tomasetti collaborated to perform Computational Fluid Dynamics (CFD) modelling of a thermal melt pool based on a oule Heated Ceramic Melter (JHCM). This forms part of an assessment of the feasibility of deploying thermal treatment for pumpable ILW. The study aims to address known risks from the perspective of gathering quality evidence, understanding uncertainty and fault, and cliff-edge scenarios. The programme will ultimately determine whether it is possible to use COTS CFD software, alongside experiments, to produce a body of evidence sufficient to support the development of a safety case satisfying UK regulatory requirements. This includes whether CFD analysis could be used to inform the scope of the more costly experimental work.

APPROACH

Sellafield Ltd has been exploring the potential application of thermal treatment for a range of waste types, through the utilisation of various melter technologies. The three melter technologies initially considered for this work were the JHCM, Cold Crucible Induction Melters (CCIM), and In-Can Melting (ICM).

The JHCM typically consists of a molten glass thermal melt pool contained within a ceramic refractory. The temperature of the pool can typically reach 1,150°C, with heating provided via electrodes. These pass an AC current through the melt, producing thermal energy in an effect known as "Joule heating". The melt pool is agitated via a "bubbler" which encourages flow and mixing of the melt.

An example schematic of a JHCM is shown in Figure 1.

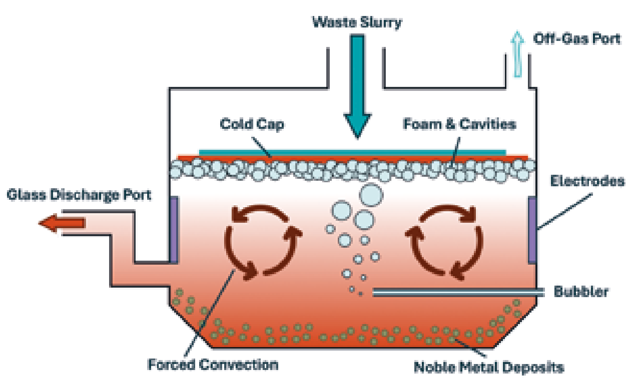

FIGURE 1: Schematic of a JHCM.

The CCIM, like the JHCM, utilises a bubbler but is comprised of a steel crucible with surrounding induction coils. Heat is produced when eddy currents are induced by these coils and can raise the melt temperature up to 2,000°C. The sides of the crucible are water-cooled and kept at relatively low temperatures (<200°C).

The ICM fills canisters with waste and, where required, glass additives, and inserts them into furnaces that close around them. The furnaces then heat up and melt the waste inside the cans. The cans themselves are then suitable for disposal.

The most important physics common to all three melters was identified. This included glass melts, heat transfer, off-gassing and particle movement. A technology-agnostic approach was decided upon and a generic model, broadly based on a JHCM, was created with agreed simplifications. The model was based on a JHCM used in recent trials for Sellafield Ltd waste, since information was available to support configuration and validation of the model.

Given the model simplifications, an exact match against the trials was not expected. However, it was anticipated that comparisons between the CFD model and trial data would support validation of specific aspects of the CFD model and provide insight into the relative significance of physics captured and omitted from the generic model.

The scope of work included single-phase modelling of the thermal melt pool, Discrete Phase Modelling (DPM) of flammable gases that could form within the pool, and DPM of solid particles within the pool. A review was also undertaken to identify further steps necessary to produce a validated model that could contribute to a body of evidence for a nuclear safety case, in line with the requirements set out in the Office for Nuclear Regulation (ONR) technical assessment guides. The CFD software utilised in this work was Ansys Fluent 2024R2.

SINGLE-PHASE MODELLING

For the single-phase analysis, a base case was created, and sensitivity studies were carried out to identify influential parameters. The aim for the base case was to match the CFD output to trial data, noting that an exact match was not expected due to the simplifications made.

The geometry was created in 2D and is shown in Figure 2. While some differences between 2D and 3D behaviour would be expected, the 2D model allowed accelerated simulation times and more sensitivity studies to be carried out. The domain was limited to the thermal melt pool, with heat transfer to adjacent surfaces and the space above the pool captured through boundary conditions.

The heating of the melt pool was achieved using Ansys Fluent's electric potential model, which enables Joule heating via the specified electrodes. Heat transfer within the model was then achieved through the conduction and convection models available.

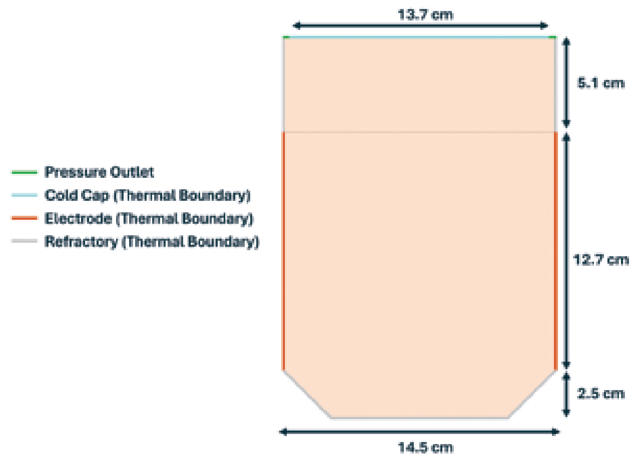

FIGURE 2: The 2D CFD model domain.

The molten melt modelled was based on the ORPLA20 glass composition, shown in Table 1. ORPLA20 is a simulated Waste Treatment and Immobilization Plant (WTP) Low Activity Waste (LAW) glass with high soda content [1]. Viscosity, density and electrical conductivity data, shown in Figure 3, was sourced for the conventional temperature range between 900 – 1200°C. This data was generated using sourced information from experiments, where possible, and extrapolation equations such as the Vogel–Fulcher–Tammann (VFT) equation.

For sensitivities performed later in the analysis, data was sourced for an additional 38 borosilicate glasses, from which two glasses were selected: LAW-Matrix 4 (LAWM4) and LAWM7 [2]. Both compositions are experimental matrix glasses developed by Vitreous State Laboratory. These glass compositions were selected to represent lowest and highest viscosity of all the glass compositions considered.

TABLE 1: The chemical composition [Wt.%] of ORPLA20, LAWM4 and LAWM7.

Chemical Component	ORPLA20 [1]	LAWM4 [2]	LAWM7 [2]
SiO_2	42.51	41.98	52.00
Na_2O	24.00	5.46	5.81
B_2O_3	8.80	13.53	6.95
Al_2O_3	6.70	3.26	5.25
ZrO_2	6.00	4.44	0.03
CaO	3.30	9.33	9.55
ZnO	2.76	4.72	1.00
Other	5.93	†17.28	†19.41

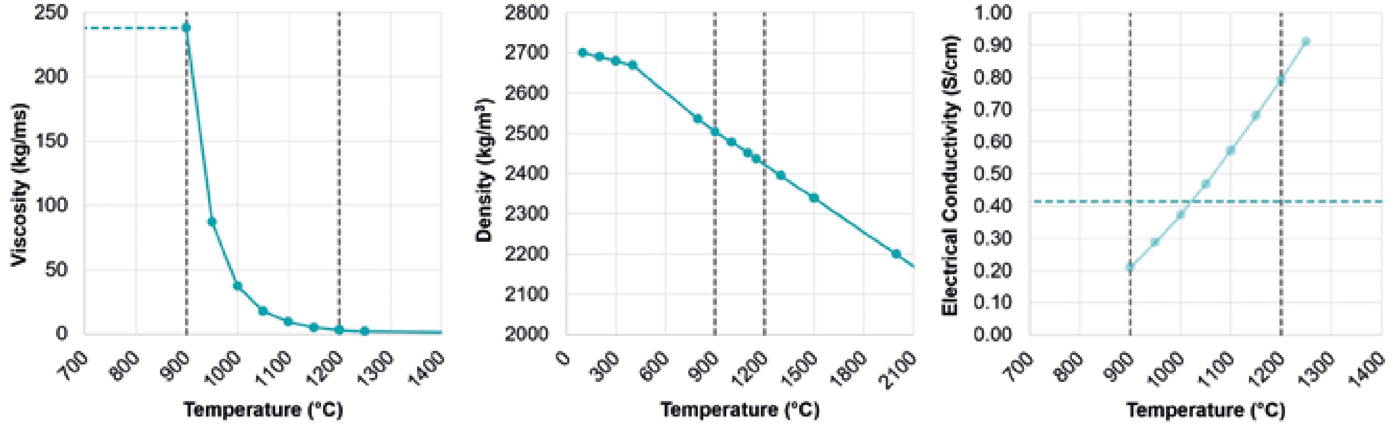

FIGURE 3: Sourced viscosity, density and electrical conductivity data for ORPLA20. The blue dotted line on the viscosity graph represents how Fluent truncates and extrapolates the data. The blue dotted line on the electrical conductivity graph represents the single value of 0.414 S/cm that was used in the model instead of the temperature-varying data shown in faded blue. The grey dotted lines in all graphs represent the upper and lower bounds of the originally anticipated temperature range of the glass melt (900 – 1200°C).

After several iterations of modelling, the electrical conductivity was fixed to a value of 0.414 S/cm based on a mean value of multiple trial glasses. Fixing the electrical conductivity to a single value prevented a positive feedback mechanism whereby a small increase in melt temperature would increase the electrical conductivity, which would increase the electrical current and Joule heating power, which would then increase the temperature. This is a known limitation of the software based on conversations with Ansys, who advised that User Defined Functions (UDFs) can be used to regulate the voltage based on the current, as done in practice.

This assumption was considered to have a minor impact on the model itself. Power distribution plots (such as Figure 4) showed that despite the constant electrical conductivity, the current still predominantly passes through the centre of the melt where temperatures are higher and where, in practice, the conductivity would be highest. If electrical conductivity were temperature dependent in the model, the power distribution would be expected to look similar.

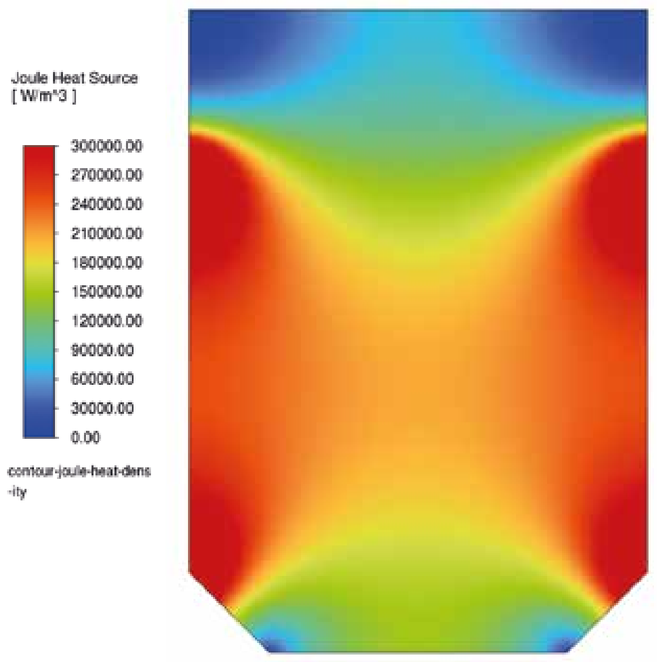

FIGURE 4: Joule Heating power distribution for the initial base case CFD model.

The voltage across the electrodes was specified to be 10.7 V, to reach the target melt temperature of 1150°C. The power input to achieve this equated to 845 W and was significantly lower than that used in trials (~5 kW, 28 V). The temperature towards the top of the melt, approximately 600°C, was also much lower than the expected melt temperature of 900– 950°C observed in trials.

These differences were likely due to the absence of the "bubbler" as shown in Figure 1, and the turbulent flow it causes within the melt pool, in the model. Turbulence would promote significant heat and mass transfer from the central and lower parts of the melt pool to the surface. This would require further investigation and a higher fidelity model to fully understand.

The calculated flow patterns in the melt pool displayed Rayleigh-Taylor instability (similar to that of a "lava-lamp"), see Figure 5. In the CFD model, most of the heat rejected from the melt pool is rejected at the melt pool surface (~90%). Engineering calculations using information from the trials found that approximately 75% of the heat input would be required to boil off water from the cold cap and raise this to the plenum temperature. In practice, further energy would be needed to heat other materials within the cold cap. Therefore, the finding from the CFD model is broadly consistent with expectations.

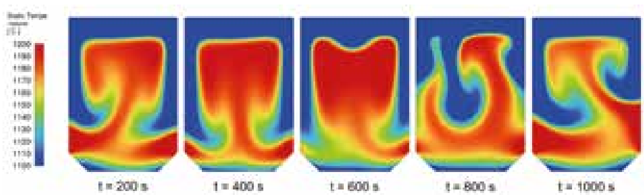

FIGURE 5: Slow convective movement of the highly viscous glass, driven by buoyancy, enables regions of differing temperature (as shown in the figure) and density to develop. A region of heated lighter glass develops below the cooler heavier glass, which results in the development of Rayleigh-Taylor instabilities i.e. a "lava-lamp" type effect.

During testing of the CFD model, viscosity was identified as a key parameter in governing the melt velocity. This in turn affects the convective heat transfer and melt temperature. Rather than adjusting only the viscosity for sensitivity studies, existing glass definitions were sought to ensure that the density and thermal properties of the melt were representative of real glasses.

As noted earlier, two glass compositions, LAWM4 and LAWM7, were selected for the sensitivity analysis [2]. These represent the glass compositions with the lowest and highest viscosities of the glasses researched.

No temperature-dependent density data was available for these except at room temperature: 2720 kg/m^3 for LAWM4 and 2660 kg/m^3 for LAWM7 [2]. The differences between these densities and the density of ORPLA20 at room temperature were assumed to be maintained over the complete temperature range of ORPLA20 density data. The final viscosity and density data used for LAWM4 and LAWM7 is compared against that for ORPLA20 in Figure 6.

When modelled, the lower viscosity of LAWM4 was seen to allow more recirculation and higher velocities to occur in the top layer of the melt. This recirculation acts to promote heat transfer from the melt in the same way a turbulent boundary layer would.

The findings from this sensitivity study highlighted the importance of accurately capturing the physical processes at the top of the melt in calculating the heat loss. This would enable meaningful studies to be performed on cold cap and plenum design, and operational parameters, in the future.

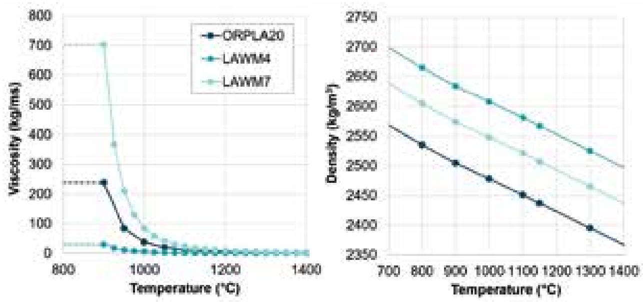

FIGURE 6: Comparison of viscosity and density data for LAWM4 and LAWM7 against that for ORPLA20.

Further studies also showed that the model was sensitive to timestep size, electrode geometry, e.g. variations in height or whether the electrode protruded into the melt vs. sitting flush with the refractory, and the depth of the pool. The average melt temperature for a given power input is sensitive to any parameter that affects the convective heat transfer to the melt pool surface from the region between the electrodes.

Given the absence of a bubbler in the generic model, the calculated melt pool flow was observed to be laminar. Under these conditions, sensitive parameters included temperature dependent melt properties and the power input / electrical conductivity. E.g. for the ORPLA20 glass used as the base case for this study, a 19% reduction in power produced a 22% reduction in average melt temperature.

A further study looked at the suitability of Ansys Fluent's pseudo steady-state solver compared to a transient solver, based on the inherently unsteady nature of the flow field demonstrated in Figure 5. The study found that temperature and velocity profiles at equivalent time points were sufficiently similar; thus, it was concluded that the pseudo-steady state method was appropriate for this level of analysis. The study also confirmed that the unsteady nature of the flow field was not an artefact of the steady-state solver.

MULTI-PHASE MODELLING – GAS BUBBLES

Flammable gas bubbles could occur within the melt pool, either through entrainment of gas by material entering the melt pool from the cold cap, or through chemical reactions within the glass melt.

In Ansys Fluent, the flow of gas bubbles or solid particles through a liquid can be modelled using either the volume of fluid (VOF) model or the DPM model, which uses "parcels" to represent a group of like particles. Each parcel can contain any number of particles, based on the parcel's given mass flow rate, density and diameter. Calculating the trajectory of hundreds or thousands of particles individually can be computationally prohibitive, so using parcels simplifies the simulation while still providing accurate results. This method was chosen for the flammable gas modelling.

For the flammable gas modelling, eighteen locations were chosen as injection sites (see Figure 7). Larger gas bubbles were initially placed towards the top of the melt pool, since bubbles of this size are more likely to be entrained from the interface with the cold cap, and smaller bubbles were initially placed towards the bottom of the melt pool.

The mass flow rate was calculated for each gas bubble based on its diameter, the density of the gas and the time step used. Initial velocities were set to zero, so that the surrounding flow of the glass melt would fully influence the particle motion. The positions of each bubble were tracked over a runtime of 60 seconds. These paths can be seen in Figure 8.

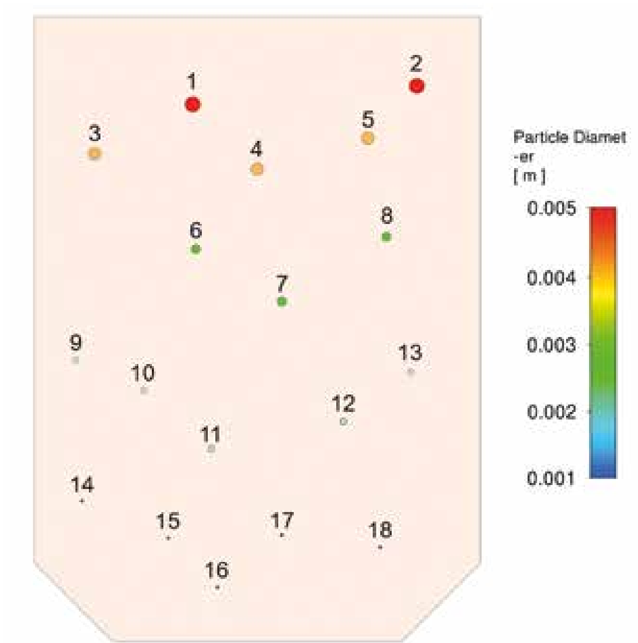

FIGURE 7: Starting locations and bubble diameters for the discrete phase in the DPM gas bubble modelling.

DPM modelling assessed the sensitivity of the gas bubble behaviour to the following parameters:

- Bubble size: The bubble diameter starting distribution was reversed so that bubbles had opposite diameters over the 1 mm to 5 mm range modelled. This was to assess the sensitivity to bubble diameter on movement through the different viscosities within the melt. The results are shown in Figure 8.
- Glass melt properties: The continuous glass melt phase was changed from the ORPLA20 results to LAWM4 or LAWM7.
- Glass melt temperature: The continuous glass melt phase was changed from the initial results with 1150°C average temperature (determined from the single-phase ORPLA20 modelling) to average melt temperatures of 900°C or 1400°C, by varying the power input.
- Drag coefficient: The default Spherical Drag Law used in the Fluent DPM model assumes that particles are smooth solid spheres. The sensitivity to this assumption was assessed by running a simulation that accounted for reduced tangential shear stress applicable to bubbles.

FIGURE 8: Bubble paths over 60 seconds for the base case (left), the bubble size sensitivity where the bubble positions were reversed (middle), and the drag coefficient sensitivity study where a UDF was used to account for reduced tangential shear stress (right).

The DPM modelling for flammable gases showed that the bubbles are strongly affected by the viscosity of the melt. They move easily through areas of low viscosity and, particularly for the smaller particles, remain suspended within highly viscous areas. Any slight changes to melt temperature, and therefore viscosity, would affect the ability of bubbles to move in the melt, with the potential for areas in the melter to change bubble capture behaviour within a timescale of minutes. The most viscous region of the melt pool occurs at the top and can result in bubbles being held in suspension underneath the cold cap (as shown in Figure 1). Although not explicitly considered in this modelling, this is likely to contribute to foaming behaviour known to occur in melters. In general, any flammable gases that escape from the melt pool would be burned off as it escapes, due to the high operating temperatures. This prevents a significant flammable atmosphere from developing and is an advantage of thermal treatment compared to alternative waste processing.

Bubble behaviour is also sensitive to diameter, with bubbles of diameter 1 mm and 5 mm displaying significant differences in behaviour. Bubbles with 1 mm diameter are strongly influenced by local flow patterns in the melt, whereas larger bubbles were only weakly affected and would rise vertically through less viscous areas of the melt (i.e. buoyancy effects dominate).

MULTI-PHASE MODELLING – SOLID PARTICLES

Particles of solid matter, typically with diameter in the range 1 μm to 1 mm, are expected to be present in the melt pool due to the nature of the feedstock. A potential challenge to the use of thermal treatment for waste vitrification is the possible accumulation of solid material within the melter, which would pose concerns regarding criticality (potential accumulation of fissile material) and processability (potential accumulation of metals causing blockages or short circuiting of the electrodes).

Both DPM models and a dynamic overset mesh method were used when assessing the movement of solid particles. DPM is better suited to particle sizes that are small in comparison to the mesh element size; the overset mesh method is better suited to particle sizes that are of the same order or larger than the mesh element size. It appeared that the overset mesh method is limited in terms of practicality for running analysis covering a wide range of particle sizes and performing many sensitivity studies. The overset mesh approach requires smaller timesteps with increasing fluid viscosity, resulting in extremely long run times. By comparison, DPM models for the same analysis setup, run in a fraction of the time (several minutes to a couple of hours) and would still yield insightful results. Other limitations of the overset mesh method include incompatibility of Fluent's Joule Heating model and deactivated mesh regions, and the interaction of particles with other solids, including walls, is not captured.

The single-phase 2D model was used to initialise the model for the DPM simulations. Nine solid particles were then added to the thermal melt pool domain, at the locations shown in Figure 9. For each simulation, all particles were of the same size and material. The positions of the particles were tracked over a 5-minute time period. Each particle type modelled was representative of particles that could credibly be present in the waste streams or generated during the thermal treatment process (such as transition or noble metals, or fissile material).

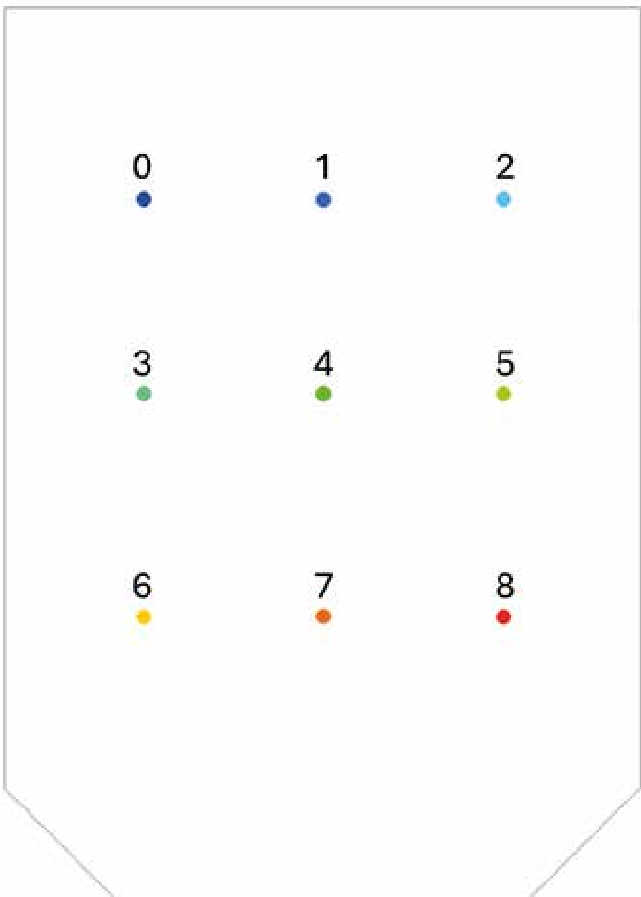

FIGURE 9: Starting locations for the discrete phase in the DPM solid particle modelling.

Figure 10 shows an example of the final particle positions for 1 µm, 100 µm and 1 mm cases for one of the particle materials modelled. Figure 10 shows that for solid particles with diameters less than or equal to 100 µm, the motion is drag dominated, with negligible difference in the particle positions after five minutes, at the end of the transient simulation. Some of the 1 mm diameter particles are not present in the right hand figure; these reached the bottom of the melt and were removed by the "trap" particle boundary condition. For these heavier particles, gravitational forces play an important role alongside drag forces.

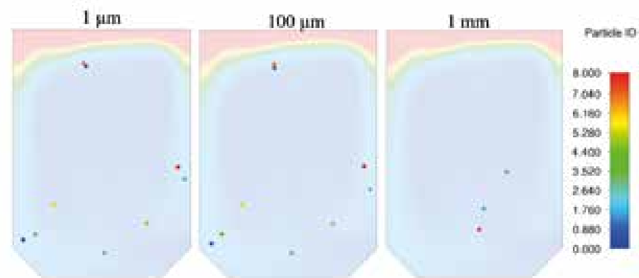

FIGURE 10: An example of final positions for particles with 1 µm (left), 100 µm (middle) and 1 mm (right) diameters.

The final particle locations indicate a potential grouping of the particles whilst in suspension. As the particles recycle, they travel downwards through the narrow flow currents at the sides of the melter (bringing the particles closer together than their starting positions). This could be due to simplifications of the model (such as lack of agitation). There may be benefit in further work to assess the sensitivity of the model to these simplifications and in running these analyses for longer and in 3D to see if more cohesive groups of particles form, which would indicate a potential for short circuiting or formation of a critical mass.

CONCLUSIONS

The initial single-phase modelling showed that COTS CFD software has potential to contribute to future safety case development. The 2D approach captured much of the physics that would be expected for a variety of melter technologies and allowed for rapid testing of modelling approaches. The work demonstrated that COTS CFD software is generally capable of modelling a simplified representation of a thermal melter with Joule heating. However, the study identified a number of expected inconsistencies between the CFD results and observations from the trials. For example, the top of the melt in the model had a temperature of 600°C as opposed to 900-950°C recorded in trials and the voltage required to reach the target melt temperature was 10.7 V in the model instead of 25-30 V in the trials. Limitations of the approach were identified, and it was concluded that the various physics omitted are likely to be significant contributors to the differences between the output from the current generic model and results from trials.

Calculated gas behaviour in the thermal melt pool aligns with expected results. The most viscous region occurs at the top of the melt pool, where it is coolest, and can result in bubbles being held in suspension underneath the cold cap.

Analysis of solid particle motion within the melt pool identified that there are cliff-edges in particle diameter and mass where gravitational forces start to dominate over drag forces, causing particles drop out of suspension and fall to the bottom of the melter. The diameter for which particles fall out of suspension depends on the particle density and may be sensitive to agitation of the melt pool and turbulence levels.

At this stage, there is significant uncertainty regarding parameters other than properties of the considered waste streams, which are themselves uncertain (see Table 2). However, the modelling performed has not identified any unsurmountable challenges and gives confidence that a higher fidelity model could be used to address these questions more fully. A higher fidelity model could also be used to develop a mechanistic understanding of thermal treatment processes, further investigate sensitivity to model and operational parameters and contribute to a body of evidence for future UK safety cases regulated by the ONR.

TABLE 2: Sensitivity to influential parameters.

Parameter	Impact	Uncertainties
Mesh resolution	Medium	Mesh resolution must be balanced against simulation run time. A mesh sensitivity study demonstrated mesh independence for the cell size taken forward to the main analysis.
Timestep	Medium	Timestep must be balanced against simulation run time. A sensitivity study informed the timestep used for the main analysis (temperature variation ~5°C).
Electrode geometry	Medium	Average melt temperature varies by approx. 7% depending on whether the electrodes are flush with the wall or protrude into the melt pool.
Melt pool depth	Medium	If the power input is maintained, a variation of up to 25°C with melt pool depth could be expected.
Power input	High	Average melt temperature (and hence viscosity) and conductivity are sensitive to power input.
Melt properties	High	Very high viscosities can cause numerical instabilities. Directly influenced by feedstock composition, which is very uncertain in some cases. Results are particularly sensitive to viscosity.
Bubble properties	High	Bubble properties and generation / entrainment rates are very uncertain. Less sensitive to composition since orders of magnitude less dense than surrounding melt.
Solid particle properties	High	Density and shape affect cliff-edge behaviours. Other parameters, such as the rate of solids entering the melt from the cold cap, precipitation rate and concentration, are very uncertain. Directly influenced by feedstock composition, which is highly uncertain in some cases.
Cold cap properties	High	Material composition, thickness, melt pool coverage and extent of foaming are uncertain (properties reported in literature vary by orders of magnitude). Directly influenced by feedstock composition, which is very uncertain in some cases. Bespoke software / functions may be required to capture complex physical and chemical processes.

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ACRONYMS

CCIM	Cold Crucible Induction Melter
CFD	Computational Fluid Dynamics
COTS	Commercial Off-The-Shelf
DPM	Discrete Phase Modelling
HLW	High-Level Waste
ICM	In-Can Melting
ILW	Intermediate Level Waste
JHCM	Joule Heated Ceramic Melter
LAW	Low Activity Waste
LAWM	Low Activity Waste Matrix
NDA	Nuclear Decommissioning Authority
ONR	Office for Nuclear Regulation
PCM	Plutonium Contaminated Materials
UDF	User Defined Functions
VFT	Vogel–Fulcher–Tammann
WTP	Waste Treatment and Immobilisation Plant

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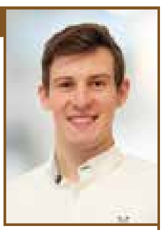
Ella Schaefer is a Project Engineer within the Applied Sciences team at Thornton Tomasetti. Ella has developed extensive experience in the nuclear industry, both during her time as a PhD researcher and at Thornton Tomasetti. Her experience includes a variety of waste management projects relating to long term storage, inspection and repackaging, in addition to looking at novel and innovative solutions for management of PCM.

SARAH SWALES

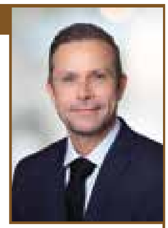
Sarah Swales is a Project Engineer within the Applied Science team at Thornton Tomasetti. She has worked on various projects including CFD modelling of gas releases, fire and gas detector layout studies and has given support to nuclear projects regarding the management of PCM.

EUAN WILLIAMSON



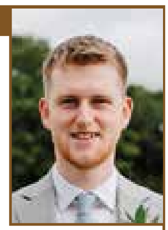
Euan Williamson is a Project Engineer within the Applied Science team at Thornton Tomasetti, specialising in the application of CFD tools to solve thermo-fluid challenges. Most recently, this has been extended to support development of solutions within nuclear waste management.

TIM ASHWORTH



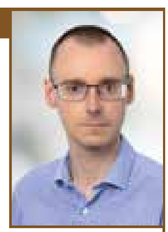
Tim Ashworth is a Principal within the Applied Sciences team at Thornton Tomasetti, with over 20 years' experience in the energy and infrastructure sector. His experience spans the full nuclear lifecycle which has allowed him to develop a detailed knowledge of the design and safety case process, including international licensing, standards, regulatory requirements and best practice.

BEN VICKERS



Ben Vickers is a Senior Engineer within the Applied Science team at Thornton Tomasetti. He has supported a range of waste management projects looking at technical issues relating to long term storage and thermal treatment.

ROB ENGLISH



Rob English is a Senior Associate within the Applied Sciences team at Thornton Tomasetti. Rob has developed a detailed understanding of major accident hazard modelling and safety assessment. His 17 years' experience includes risk assessment and CFD analysis to inform safety studies for nuclear storage and decommissioning facilities, and other energy facilities, at multiple stages of project and waste lifecycles.