Validation of the Modelling of Corrosion Driven Expansion in Grouted Wasteforms – 16125

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ABSTRACT

One of the current preferred solutions for the disposal of Intermediate Level radioactive waste in the UK is grout encapsulation inside steel boxes for long term storage. These boxes are then to be entombed in a Geological Disposal Facility once one is available. However, both prior to and during geological disposal, waste contents can react with the water present in the encapsulant grout and begin to corrode. This corrosion product occupies a larger volume (by several hundred percent) than the original material and the corrosion occurs over the course of decades and centuries, long after the encapsulant grout has set and hardened. The expanding waste then creates stresses in the encapsulant causing both it and the surrounding box to deform and, in extreme circumstances, and after long times, for the structural integrity of the box to fail.

This behaviour needs to be quantified before the box can be approved for use as any excessive deformation could lead to a loss of containment or, since the boxes are stacked on top of each other, to a significant accident in the stores. Due to the long timescales involved, physical testing of the phenomenon in full scale is impossible. Instead, a combination of chemical modelling and finite element analysis is used to predict the extent of the corrosion in the waste and its effect of the integrity of the box.

There are a number of difficulties in modelling the corrosion-driven expansion and subsequent deformation of the boxes. Although the corrosion occurs over a very long time scale, the event is highly non-linear and dynamic. All of the material models, including the steel and grout are non-linear. The deformation is in the order of 10s of centimetres, well beyond the static elastic range. Finally, the components must be allowed to move relative to each other which involve a lot of part to part contacts. This means that simple static modelling, which would solve quite quickly, cannot be used. Instead a dynamic analysis code, LS-DYNA, has been used to expand the product over time to simulate the corrosion-driven expansion. This software is generally used for modelling car crashes or scenarios where waste containers have been dropped. The analyses therefore include a significant inertial component.

This paper will detail the NNL's approach to modelling this long-term, quasi-static phenomenon in the dynamic, impact oriented software code LS-DYNA. It will cover

the problems inherent in this approach, the errors that it creates as well as the tests and solutions that NNL worked on in order to overcome them and be confident that the solution could be validated.

This work will ultimately be used to determine the maximum inventory which can be stored in each box based on the waste content and the potential extent of expansion as well as any modification that could be made to the box design or the processing streams that may improve the storage solution.

INTRODUCTION

The long term storage of nuclear waste is a significant challenge for the industry and society in general. Generally, the plan is for waste to be encapsulated, stored in boxes and these boxes stored in various sites either above or below ground. The most common encapsulant used is a grout matrix that can be poured over the waste in the boxes and then allowed to set. This provides both a physical barrier to the waste movement and radiation shielding.

However, many types of waste will tend to react with the water present in the grout and begin to corrode. This corrosion causes an expansion of the waste which can threaten to crack the grout and if the extent is great enough could threaten the integrity of the box as well.

However, creating the data needed to make sound decisions is very difficult as there is no prior experience of dealing with this type of waste over the centuries for which it will be stored. Furthermore, experimental data is difficult to come by for the same reasons. Therefore, a modelling approach is taken.

Finite Element Analysis can be used to predict how the encaspulant and package will perform when placed under strain generated from the corrosion driven expansion of the waste. This creates its own problems due to the nature of the problem and the nature of the software available to solve it.

METHODS

In modelling there are generally two forms of solver, implicit and explicit. Implicit is generally the most common and is used for modelling static/quasi-static phenomenon such as loading under gravity. Explicit solvers are generally used for highly dynamic, non-linear phenomenon such as modelling car crashes. For implicit/static analysis the NNL uses Ansys [1] and for explicit/dynamic analysis NNL uses LS-DYNA [2] supported by the Oasys Software Suite [3].

Below is a consideration of how each of these pieces of software could be used to model the corrosion expansion and the problems that each poses.

Ansys

Ansys is well suited to modelling the sort of long term, low strain rate effects that would be seen in the corrosion expansion. Given the constrained nature of much of the package, a static solution could be found where the strain in the grout is balanced by the strain in the steel walls.

Unfortunately, the long term aspects are the only positive of using a static code such as Ansys.

Firstly, all of the materials in the package are non-linear, particularly the encapsulant grout. Whilst Ansys can solve using non-linear materials, the implicit solver method is not ideal due to the long solve times required. There is also the non-linearity involved in large deformations which can be in the order of 200-300mm.

Secondly there is the issue of contacts. The waste may be held within a basket or bin, which is within a liner filled with grout which is itself within another box. Even a simple consideration gives several layers of contacts that need to be defined. Again, whilst this can be done in Ansys, both the set up time and solve time are long.

Finally, there is the issue of additional regulatory requirements such as impact assessment of the deformed packages. Ansys is unsuited for this as a standalone package though it is recognised that an Ansys DYNA implementation is available.

LS-DYNA

LS-DYNA is well suited to many of the aspects of the modelling that made Ansys unsuitable; it is designed specifically to model highly non-linear deformations; it handles non-linear materials very well and is intrinsically geared towards element failure and allows the additional impact modelling to be carried out with little effort to transfer the data. LS-DYNA is the software that the analysis was actually carried out in.

However, due to the original purpose of the software as a modeller for car crashes, it has some limitations.

The ultimate problem is the timescales involved. Crashes typically occur over the course of a few tens of milliseconds whereas the corrosion expansion takes place over decades and centuries. On the face of it the solution seems simple; increase the length of the analysis. However, this does not work because of the explicit nature of the solver. In order to properly calculate how the stress propagates in a dynamic way over such a short time scale, the time increments in the model must be such that the stress waves (which travel at the speed of sound) must not be able to cross the distance between the nodes of the smallest element. This ensures that all stress responses are captured as they occur and all nodal positions can be updated correctly within the same timestep. This invariably means that individual timesteps can be 10E-6 of a second. Calculating the deformation occurring over a 100year timescale with timesteps of this size is impossible; NNL generally find it takes 12-24 hours to model 100milliseconds. By the time the model had finished running the actual process would have been completed thousands of years before.

The solution to this is to use time scaling; to apply the loading to the model more rapidly than in reality. In order to allow the analysis to finish within a day or two, an analysis time of 0.1secs is used. This means applying the corrosion expansion millions of times more quickly than would happen in reality. It therefore also means introducing millions of times more kinetic energy into the system.

This is the issue that arises then; how to separate deformation caused by expansion driven stresses from deformations caused by the kinetic energy due to applying the load so quickly.

Despite being primarily an explicit/dynamic code LS-DYNA does have an implicit static solver. DISCUSSION

Damping

In order to reduce velocities in a model, numerical damping can be applied. In LS-DYNA there are two general types of damping; stiffness based and mass based. Stiffness based damping is generally useful for removing unwanted oscillations from systems at higher frequencies. Mass based damping is more useful for the type of behaviour in the expansion system so this is what has been used.

Mass based damping works by artificially increasing the mass of individual nodes during the calculation of accelerations. This has two effects, it slows down all velocities and deformations but it also effectively slows down stresses as they pass through the material.

The problem with this is demonstrated in the model shown in Figure 1.

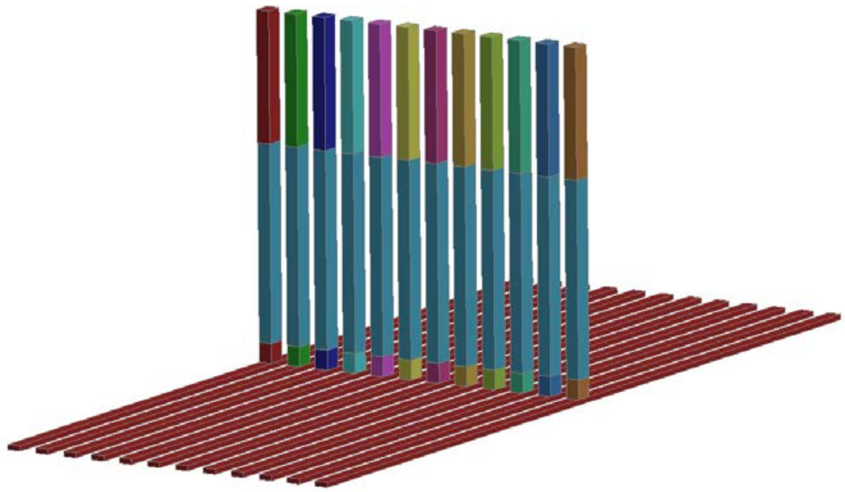

Figure 1: Simplified stick model using various grout damping

Figure 1 shows a series of bars which represent a simplified model of waste (in light blue) encapsulated with grout (various colours) resting on a steel box base (red). The waste is set up to expand at the same rate as in the actual models and the proportions of waste to grout to steel are the same. All material properties are the same as well. The most significant simplification is the lack of box side walls and grout on all sides of the waste.

Each bar has a different value of mass damping applied to the grout portion starting with the highest on the left and reducing down to zero on the right.

The results in Figure 2 show that, as would be expected, increased damping leads to reduced deformation both up and down. What can also be seen when taking a closer view is that very high damping causes significant compression of the grout (Figure 3). This occurs because the damping prevents the nodes at the top of the ‘grout’ from moving quickly enough in response to the stresses in the elements below it.

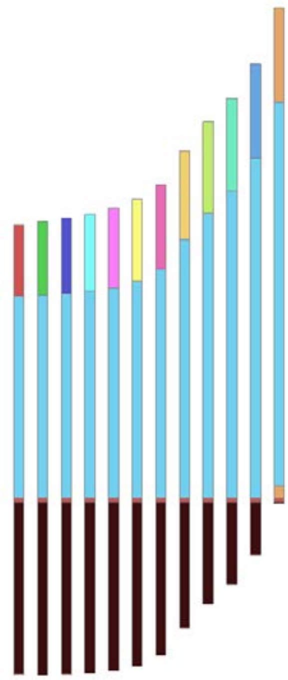

Figure 2: Expansion deformation at various damping values from high (40000) on the left to zero on right

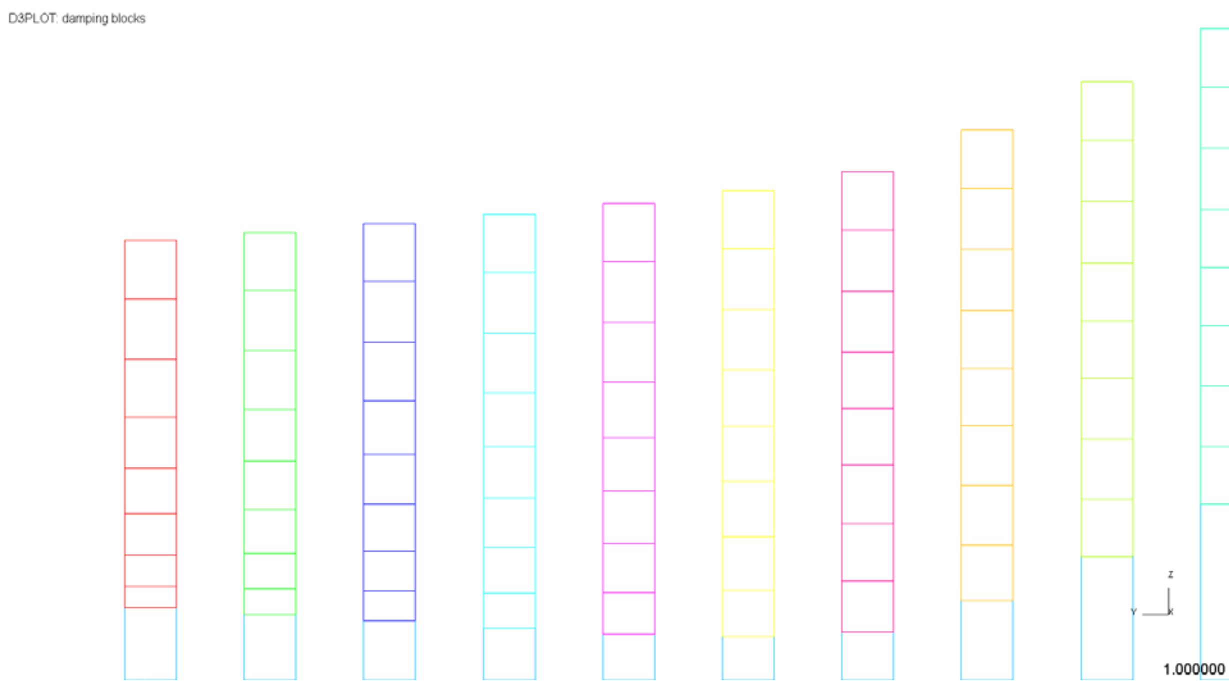

Figure 3: Compression of grout at high damping due to inertial loads

Figure 4 shows a plot of the height of the grout blocks over time. It shows that there is a significant difference between the damping values. In the long term scenarios that need to be modelled, it would be expected that there would be no compression of the grout as the deformation would occur so slowly that any stresses would have time to propagate. Figure 4 also shows the issue of inertia as the height of the undamped block actually increases.

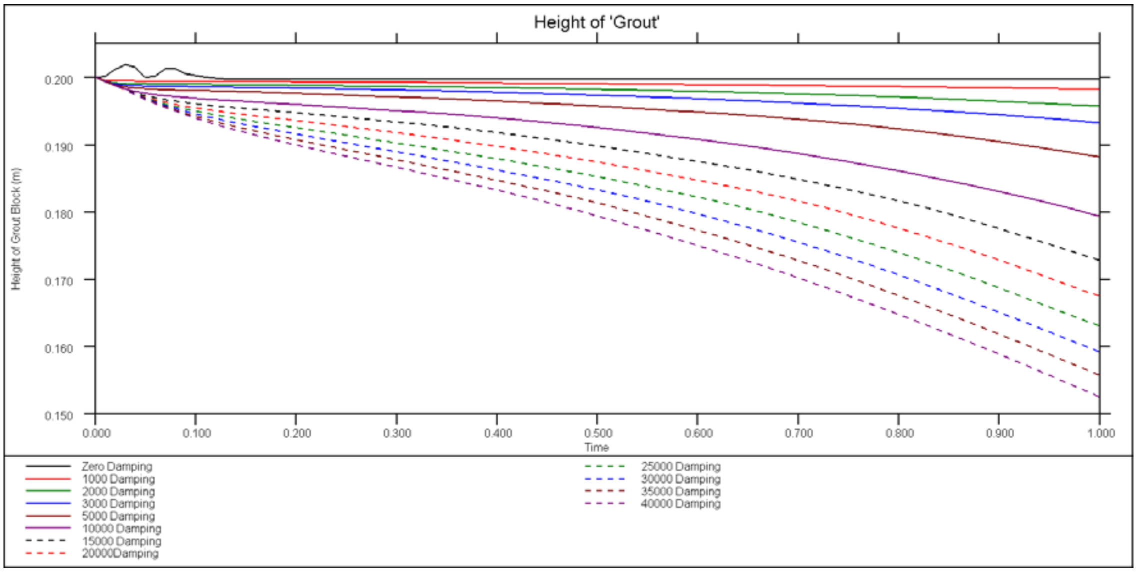

Figure 4: Height of grout in stick models

This demonstrates the problem with using this solution; choosing a value of damping which will sufficiently reduce the inertial effects of time scaling without over damping the analysis and reducing the deformation. This problem is further complicated by project constraints; time and money cannot necessarily be spent to test every model for the correct damping factors. And even if they were, there are no experimental results to compare against to validate the model. Therefore, the behavior must be verified against simple well known problems a priori.

Two routes were considered to solve this problem; to allow the analysis to continue running after the expansion had finished or to reduce the damping to very low values and consider the inertial deformation a conservatism. The first was trialed but the additional time required for stresses to completely relieve was considered too long and delayed decision making by too much. The second was rejected both because it led to deformations that were too high and a risk of tailoring the model to produce the desired results.

Without any experimental data, a method was needed of obtaining long term modelling results without the real time costs involved.

Implicit

Due to the large time scales involved the corrosion expansion that is being modelled can be considered a quasi-static phenomenon. As stated above, the problem with treating it as such is that most quasi static problems are assumed to be fairly linear.

Following several of the analyses described above, the bar model was modified to work with the LS-DYNA implicit solver. No material properties were changed but the element type was changed to be more implicit friendly.

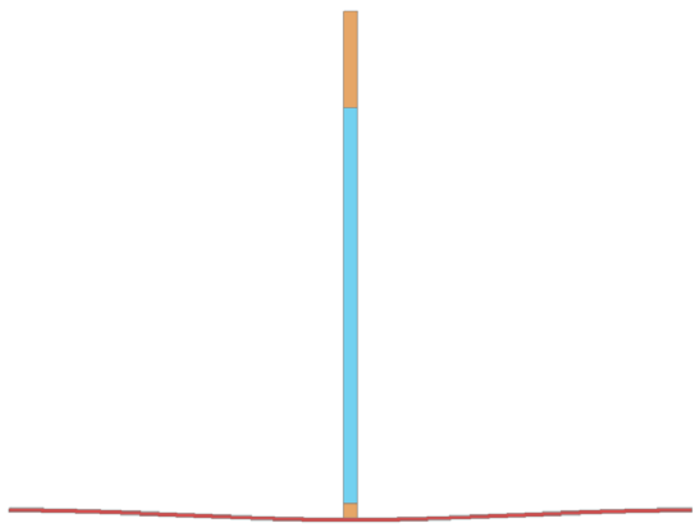

Figure 5: Deformation in an implicit analysis

The results (Figure 5) show that there is no compression of the grout – something that would be expected when the deformation occurs slowly enough on a free surface. What the results also show is that the majority of the deformation is upwards with only enough downward movement to account for the weight of the column. This is a point which differs from the dynamic analyses (with all damping values). As Figure 2 showed, the dynamic analyses show varying levels of up/down movement depending on the damping value.

Unfortunately, the implicit result runs counter to current thinking on corrosion driven expansion. Small scale trials and previous modelling work have shown that there is often very large local deformation. When the metal corrodes it does so very locally, molecule by molecule. The expansion happens in such a concentrated area that the force is not enough to move the bulk material upwards but can displace and deform the material near, or in this case, below it. This causes a gradual downwards deformation over a larger area as the waste corrodes as a whole. The difficulty is in determining how much downward movement there is compared to upwards.

This will be determined by the relative stiffness of the material above and below the expanding material. In the simple 'stick' model shown in previous figures the only constraints on the expansion were gravity and the lower metal plate. Therefore the majority of the expansion is upwards where there is no material.

However, in a more complicated model designed to mimic the grout surrounding the expanding material, a different result is seen. Figure 6 shows how the grout in the previous models has been extended to encase the expanding material in a slice.

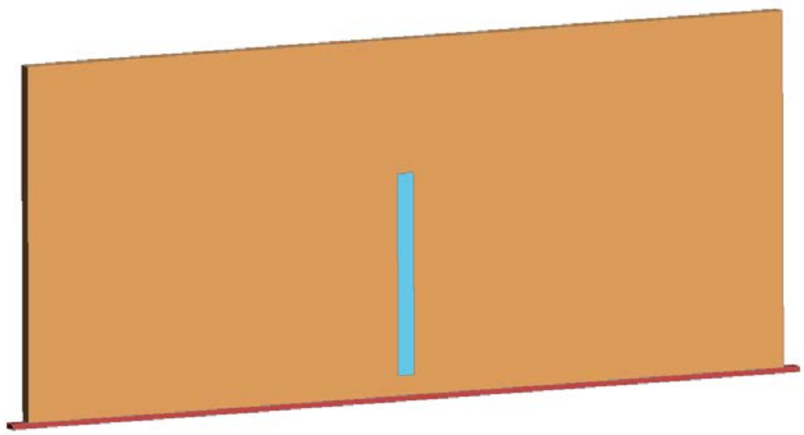

Figure 6: Implicit model with extended grout

Intermediate plots of the deformation (Figure 7) show that in this case the path of least resistance is downwards as the combined stiffness of the metal plate and small amount of grout is less than the significant amount of grout above (Figure 7 (a)). However, once the grout begins to crack the deformation then moves upwards as the free surface offers less resistance (Figure 7 (b) and (c)).

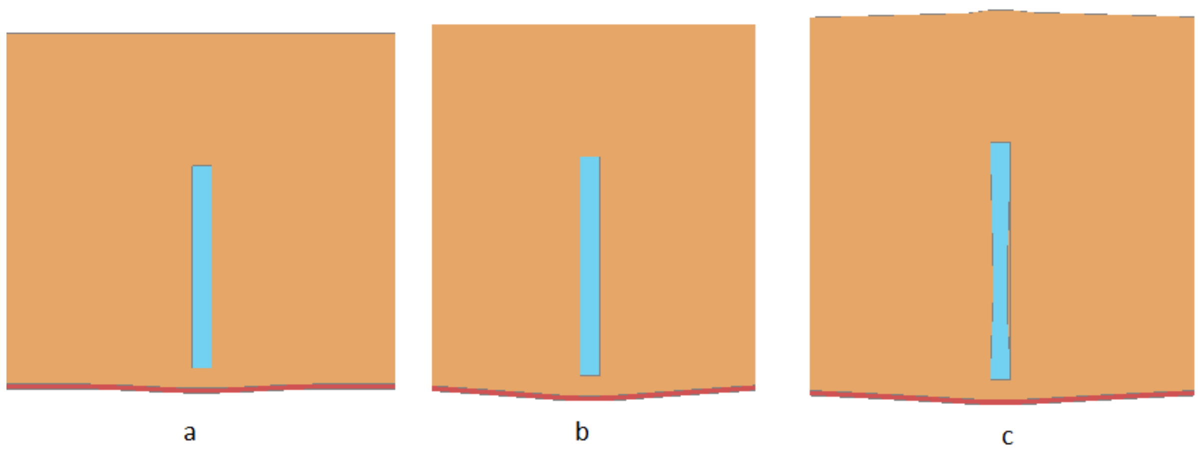

Figure 7: Deformation of the grout before (a), during (b) and after (c) cracking

When this transition occurs will depend on the formulation of grout, the arrangement of the waste and how the cracks propagate over 100s of years. Predicting the cracking alone is a significant challenge and doing so in a sensible project timescale and cost would not be feasible.

Final Choice

Despite the uncertainties inherent in only using a modelling approach to determine the expansion behaviour, NNL believe the above work gives enough technical underpinning to choose a value of damping which will create the conditions of a long term dynamic analysis.

Without further experimental work, the simplified implicit analysis is used as the reference case and a damping value of 1000 is chosen. This should give significant reductions in kinetic energy and velocities while having an acceptably small effect on deformation and run time.

It should be noted that small scale expansion trials are ongoing but were not ready to be presented in this paper. The results of these trials will be used to validate the modelling approach presented here.

CONCLUSIONS

NNL has investigated ways to model long term dynamic, non-linear corrosion driven expansion using the LS-DYNA software. The following conclusions are drawn:

- Damping is required in order to remove inertial components of deformation when modelling long term phenomenon.
- High levels of mass damping remove inertia but require additional setting time in order for trapped stresses to release and further deformation to occur.
- Different levels of damping did not have a significant effect on overall deformation once a final deformation value was reached.
- Damping levels which are too high prevent equilibrium being reached as the forces driving the deformation asymptote towards zero.
- Relatively low levels of damping are needed to replicate a static solution (<1000).
- Work is ongoing with small scale physical trials. The results of these and comparative modelling will increase the confidence in the larger scale modelling work.

Acknowledgements

The work presented in this paper is funded by Sellafield Ltd in support of their long term disposal research and development efforts.

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