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MODELING THE TEMPERATURE IN SDU 6 DURING FILLING WITH CEMENT-FREE GROUT

EXECUTIVE SUMMARY

An ANSYS® Fluent® model has been used to simulate one year of filling SDU 6 with cement-free grout. A run with an aggressive pour schedule consisting of seven 12.3-day pours separated by 46.6-day idle periods, resulting in 22.5 feet of grout being poured, predicts maximum grout and air temperatures of approximately 76 and 71 °C, respectively. The maximum temperatures for the second year of pouring are estimated to be about 5 °C higher. These temperatures exceed the Documented Safety Analysis (DSA) limits. However, the lack of convection in the SDU vapor space means that the model tends to overpredict temperatures. A less aggressive, biweekly pour schedule (70.35 h pouring + 265.65 h idling [nominal]) results in lower temperatures while maintaining the same annual grout pouring rate. The predicted maximum grout and air temperatures are 60.4 and 58.0 °C, respectively, which are within the DSA limits.

INTRODUCTION

A transient ANSYS® Fluent® model of the temperature inside a Saltstone Disposal Unit (SDU) during grout pouring has been developed at Savannah River National Laboratory (SRNL) [1]. This model is now owned by Savannah River Remediation (SRR) [2]. One purpose of this model is to check whether the temperature in SDU 6 will exceed the values assumed in the documented safety analysis (DSA) when SDU 6 is filled with cement-free grout.[1] These values are 65 and 75 °C for air and grout, respectively [3, pp. 3-21 & 3-22].

The results for SDU 6 in [1] cover two 12.3-day pours separated by a 46.6-day idle period. This is insufficient to determine the temperature resulting from several pours. In addition, an error in the ambient temperatures used for part of the model has recently been discovered. While the period modeled in [1] is unlikely to be significantly affected, the ambient temperature in the model would be too low during the summer months, which would likely result in the SDU temperature at that time being significantly underestimated. There were also minor errors in the grout density, specific heat capacity, and thermal conductivity for at least part of the SDU 6 run (the values in the model files did not match the values in the report). However, these are not expected to have a major effect on the

[1] Also referred to as 60/40 grout, since it consists of 60% blast furnace slag and 40% fly ash.

results. Note that the SRNL results were generated using Fluent version 6.3 on a Linux machine, whereas the current results were generated using Fluent version 19.2 on a Windows machine. It is speculated that this difference is responsible for the minor differences seen between the SRNL and SRR benchmarking results [2].

This memo describes runs of the SDU 6 model by SRR covering seven 12.3-day pours, with grout being poured 24 hours a day, separated by 46.6-day idle periods (approximately one year of operations) [4]. The grout pour-rate is assumed to be 150 gpm [4]. As the average inner diameter of SDU 6 is 375 ft [5], this means that 3.2 ft of grout are added per pour, or a total of 22.5 feet. This would result in SDU 6 being approximately half filled (interior height of vault is 43 ft [5]; however, note that currently the grout height is limited by the DSA to 21.7 ft [3, p. 4-16]). This pour schedule results in 16.5 Mgal of grout being poured per year, corresponding to 9 Mgal/yr of decontaminated salt solution (DSS; using a nominal value of 1.76 gal of grout per gallon of DSS [6]). Runs with shorter duration pours, but the same average annual grout pouring rate, are also investigated. All runs presented in this report use the correct ambient temperature data and grout properties.

MODEL

Inputs

The model is described in [1]. The details of the pours were obtained from Appendix A-4 of this reference and added to the C code that calculates the heat of hydration for each grout layer. The heat of hydration is for 60/40 grout with Lehigh slag and "New SWPF" salt solution simulant.

In the original model, if a grout layer took time Δt to be poured, it was assumed to be "born" at an age of $\Delta t/2$ [1]. This means that, for a typical value of $\Delta t = 12$ h, the heat produced in the first 6 h of curing was neglected. For the current runs, the entire heat of hydration curve was used.

The grout properties are from Table 2-1 in [1] (which are taken from [7]). These are reproduced in Table 1. The time-stepping and convergence tolerances used for the current runs are as recommended in [2].

The ambient temperature data for 2015 through 2017 (specifically, the daily maxima and minima measured in A area) were obtained from the SRNL Atmospheric Technologies Group's website (https://weather.srs.gov/weather/climate_data). The data were then averaged on a day-by-day basis (to simplify the calculation, 29 February 2016 was ignored – this is expected to have a negligible effect on the results). These averaged temperatures were then used to create the C code that calculates the ambient temperature as a function of time (see [1, §2.4] and [2, §3.1]).

Quantity	Units	Value
Density	kg/m^3	1710
Specific heat capacity	J/kg/K	1960
Thermal conductivity	W/m/K	0.74

Table 1. Properties of the SDU 6 grout.

Checking the Solver Settings

To check the solver settings (specifically, the time step size and the convergence tolerances), the model was run from $t = 0$ with the original, incorrect, ambient temperature and grout properties. The results from this run are in excellent agreement with the results reported in [1] (see Figure 1). This implies that the solver settings are not leading to inaccurate results, and that the results reported below are reliable.

Verifying the Ambient Temperature in the Model

Because of the ambient temperature error in the original model, the calculation of the ambient temperature, T_{amb}, in the current model was verified. This temperature cannot be directly output from the Fluent run. However, it can be inferred from the temperature of the top concrete surface of the SDU, T_{S}, and the heat flux from this surface, F, both of which can be output by Fluent.

The upper surface of the model is cooled by convection and radiation [1]. Therefore,

$$F = h(T_{\mathrm{S}} - T_{\mathrm{amb}}) + \epsilon\sigma\left(T_{\mathrm{S}}^4 - T_{\mathrm{amb}}^4\right), \qquad (1)$$

where $h = 9\ \mathrm{W/m^2/K}$ is the heat transfer coefficient, $\epsilon = 0.9$ is the emissivity [1], and σ is the Stefan-Boltzmann constant. The two terms on the right-hand side of the Equation (1) represent convective and radiative cooling, respectively. Given F and T_{S} from the Fluent output, Equation (1) can be solved for T_{amb} (see Appendix for details).

Figure 2 compares the temperatures inferred from the Fluent output with the ambient temperature data used as inputs. The measured minima and maxima are assumed to occur at midnight ($t = 0, 24, 48, \ldots$ h) and noon ($t = 12, 36, 60, \ldots$ h), respectively. The blue curve representing the ambient temperature in the model passes through all the input data points, implying that the ambient temperature calculation has been correctly implemented in the model.

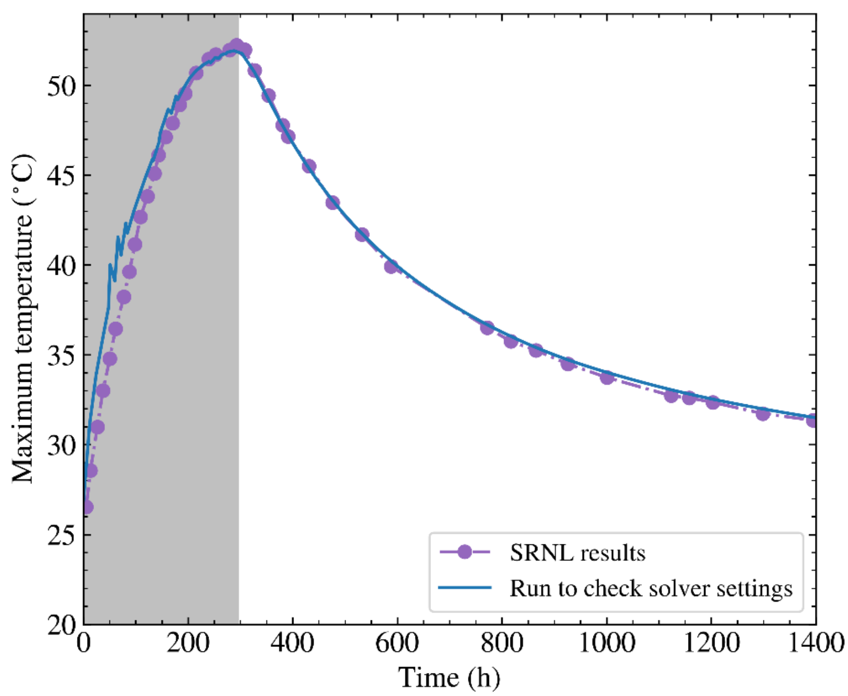

Figure 1. Results from run for checking solver settings, compared with results from SRNL [1]. The gray band indicates the timing of the first grout pour.

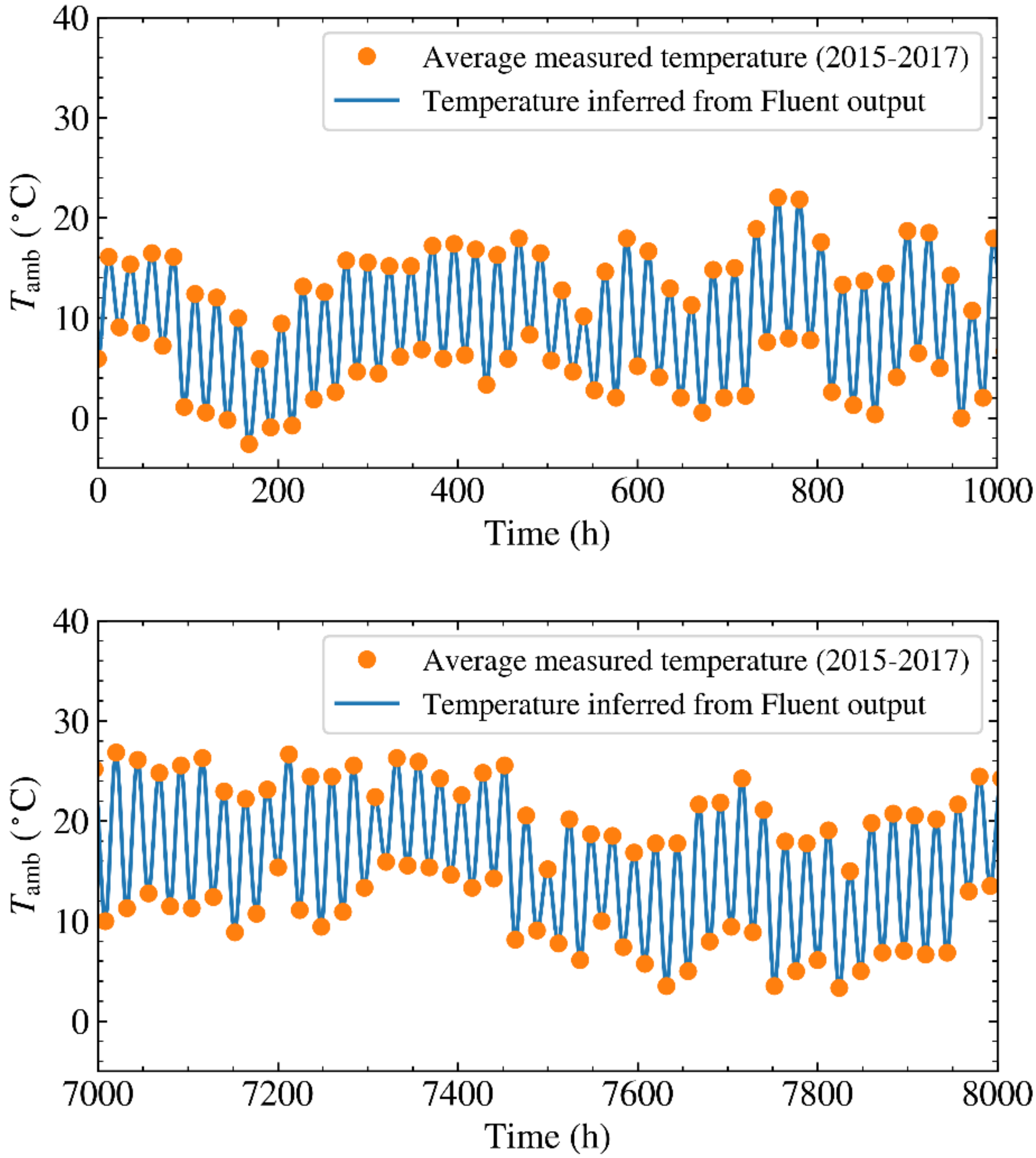

Figure 2. Ambient temperature inferred from Fluent output (blue curve), compared with the average measured temperatures used as inputs (orange circles), for two representative 1000-hour periods.

RESULTS

Figure 3 shows the maximum predicted grout and air temperatures in SDU 6 as functions of time, for one year of pouring of cement-free grout. For this run, the pouring is assumed to begin on January 1st. The maximum temperatures during each pour are shown in the second and third columns of Table 2. Note that the maximum grout temperatures at the ends of the first and second pours are higher than those reported in [1] (52 and 56 °C, respectively). This is because the full heat of hydration curve is used here, and so more heat is added to the grout.

The maximum grout temperatures generally occur slightly below the grout surface. The maximum air temperatures are generally ≈5–6 °C lower than the corresponding maximum grout temperatures, and occur at the bottom of the vapor space, where the air is in contact with the grout surface.

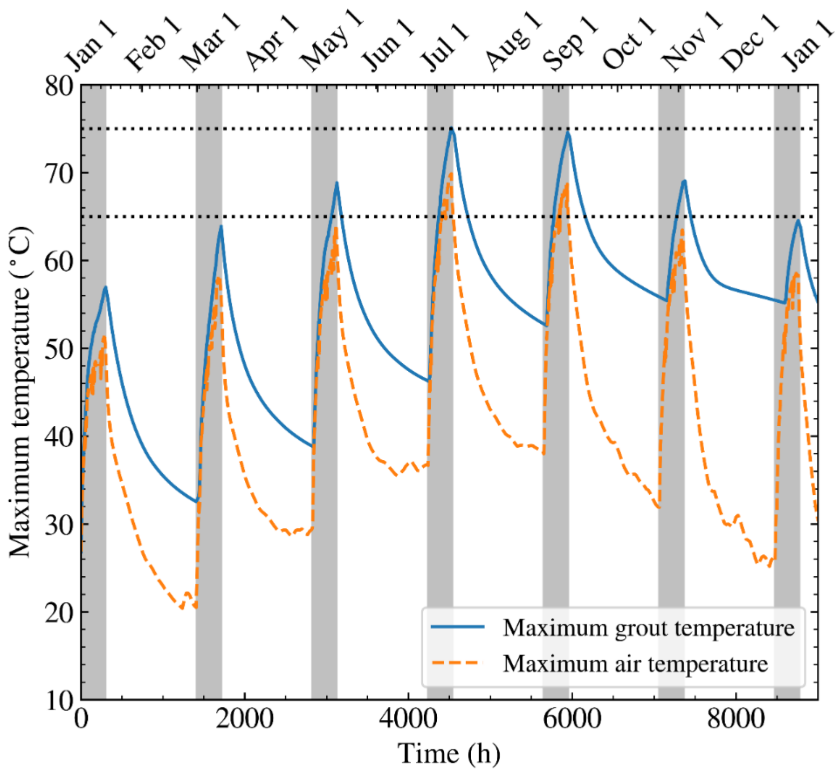

Figure 3. Maximum grout temperature (blue solid curve) and maximum air temperature (orange dashed curve) in SDU 6 during one year of pouring cement-free grout. The pouring is assumed to start on January 1st. The gray bands indicate the timings of the pours. The horizontal dashed lines indicate the maximum allowed grout and air temperatures (75 °C and 65 °C, respectively [3]).

Pour	Run starting on Jan 1st		Run starting on Jul 1st	
	Max grout temp (°C)	Max air temp (°C)	Max grout temp (°C)	Max air temp (°C)
1	57.0	51.6	72.6	68.2
2	63.9	58.3	72.7	66.2
3	68.8	64.1	67.9	62.2
4	**75.1**	**69.9**	62.1	56.2
5	74.6	68.7	62.6	56.9
6	69.1	63.5	70.3	64.9
7	64.5	58.6	**76.1**	**70.9**

Table 2. Maximum grout and air temperatures (in °C) reached during each grout pour. Overall maximum temperatures are highlighted in bold.

The maximum temperatures at the end of the fourth pour are 18 °C higher than those at the end of the first pour. This is mainly due to the increase in the ambient temperature between January and July – the average ambient temperatures during the first and fourth pours were 7.9 and 28.1 °C, respectively. After the fourth pour, the peak temperatures start to decrease as the model heads back into winter. The peak temperatures at the end of the seventh pour are ≈7 °C higher than those at the end of the first pour, despite these pours occurring at similar times of the year. The higher temperatures during the later pour are partly due to the average ambient temperature being higher (12.6 versus 8.6 °C), and partly due to the underlying layers of warm grout. The overall maximum temperatures occur at the end of the fourth pour: 75.1 and 69.9 °C for the grout and air, respectively.

Because the temperatures in the SDU depend strongly on the ambient temperature, a pouring campaign that started at a different time in the year would predict different temperatures as functions of time, and possibly result in a different overall maximum temperature. Figure 4 shows results from a run in which pouring is assumed to being on July 1st (i.e., 6 months later than in Figure 3). The maximum temperatures during each pour are shown in the fourth and fifth columns of Table 2. The peak temperatures are similar for the first and second pours, are lowest for the fourth pour, and increase up to the seventh pour, as the model heads from summer to winter back to summer. The overall maximum temperatures occur at the end of the seventh pour: 76.1 and 70.9 °C for the grout and air, respectively. The peak temperatures at the end of the seventh pour are a few degrees higher than those at the end of the first pour, despite these pours occurring at similar times of the year. The average ambient temperatures are similar for the two pours: 29.0 °C (first) and 28.1 °C (seventh).

Figure 5 compares the results obtained with the cement-free (60/40) grout's heat of hydration with results obtained using the heat of hydration for the current cement-containing grout.[2] The cement-free grout has a higher heat of hydration and, as expected, results in higher grout temperatures (by about 5 °C at the peaks) and air temperatures (by about 7 °C at the peaks) than the current grout formulation.

[2] Also referred to as 45/45/10 grout, since it consists of 45% blast furnace slag, 45% fly ash, and 10% ordinary Portland cement. The heat of hydration used here is for 45/45/10 grout with Holcim slag and "Tank 50 CY2013 Q1–Q3" salt solution simulant. This mimics the grout that was poured into SDU 2A.

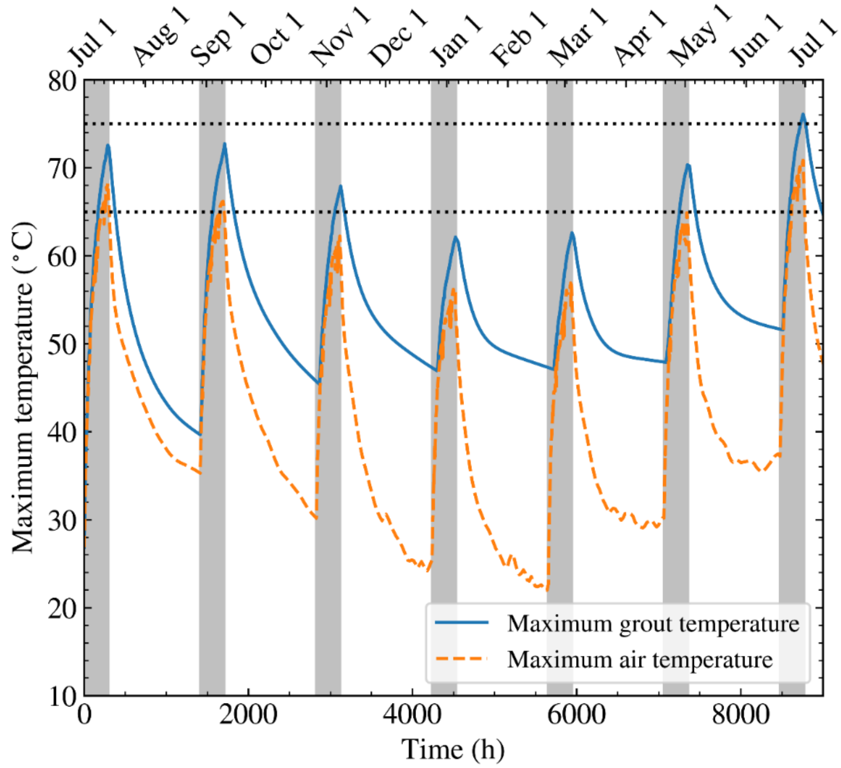

Figure 4. Same as Figure 3, but with grout pouring starting on July 1st.

It should be noted that the pour schedule modeled here is very aggressive, in that it assumes an average DSS feed rate of 9 Mgal/yr, and long, continuous pours. Shorter-duration pours would result in the newly poured layers having larger surface area-to-volume ratios, and thus cooling more efficiently. Hence, lower peak temperatures would be expected, while maintaining the same annual grout pouring rate.

To test the effect of the pour schedule, two additional schedules were modeled: a weekly schedule with 35.17 hours of continuous pouring followed by 132.83 hours of idle time, and a biweekly schedule with 70.35 hours of continuous pouring followed by 265.65 hours of idle time [4]. In practice, because the model had already been gridded for the long-pour schedule, the pour durations were 36 or 34 h for the weekly schedule and 72 or 70 h for the biweekly schedule. In all cases, the idle time was chosen so that the next pour started exactly 1 or 2 weeks (as appropriate) after the start of the preceding pour. Assuming a grout pouring rate of 150 gpm [4], these schedules both result in an average of 16.5 Mgal of grout pouring per year (the same as the long-pour schedule modeled above).

The results from these runs are shown in Figure 6. Within each time period bound by the starts of the long pours (i.e., by the gray lines in Figure 6), the biweekly pour schedule results in a maximum grout temperature 12–16 °C lower than the long-pour schedule, despite the fact that, on average, the same amount of grout is poured in both cases (Table 3). The maximum grout and air temperatures are 60.4 and 58.0 °C, respectively, and occur around August 1st. The weekly pour schedule (which only has data available up to 4700 h) predicts temperatures a few degrees lower.

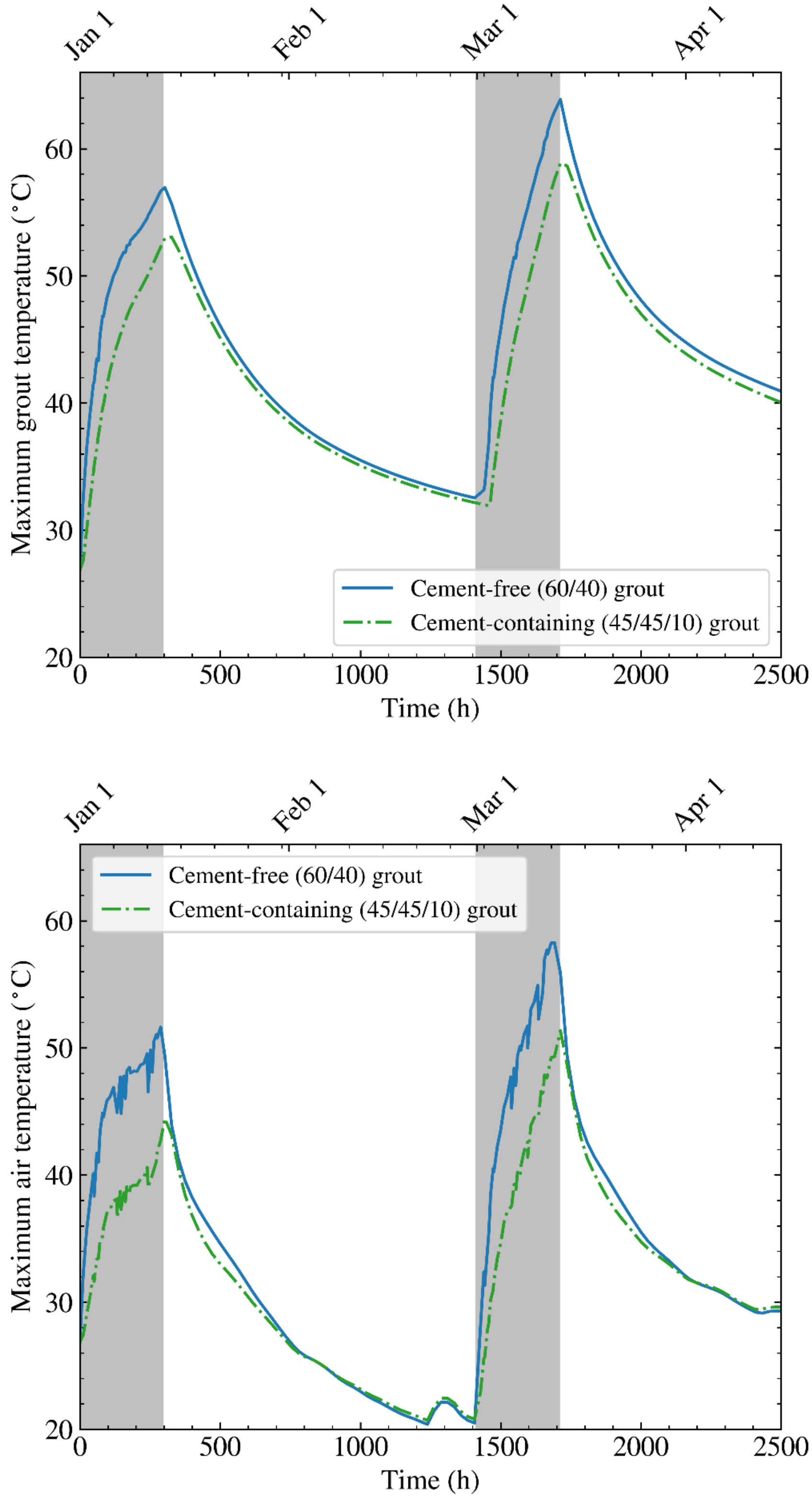

Figure 5. Comparison of the maximum grout (upper) and air (lower) temperatures in SDU 6 predicted for cement-free (60/40) grout and for the current cement-containing (45/45/10) grout.

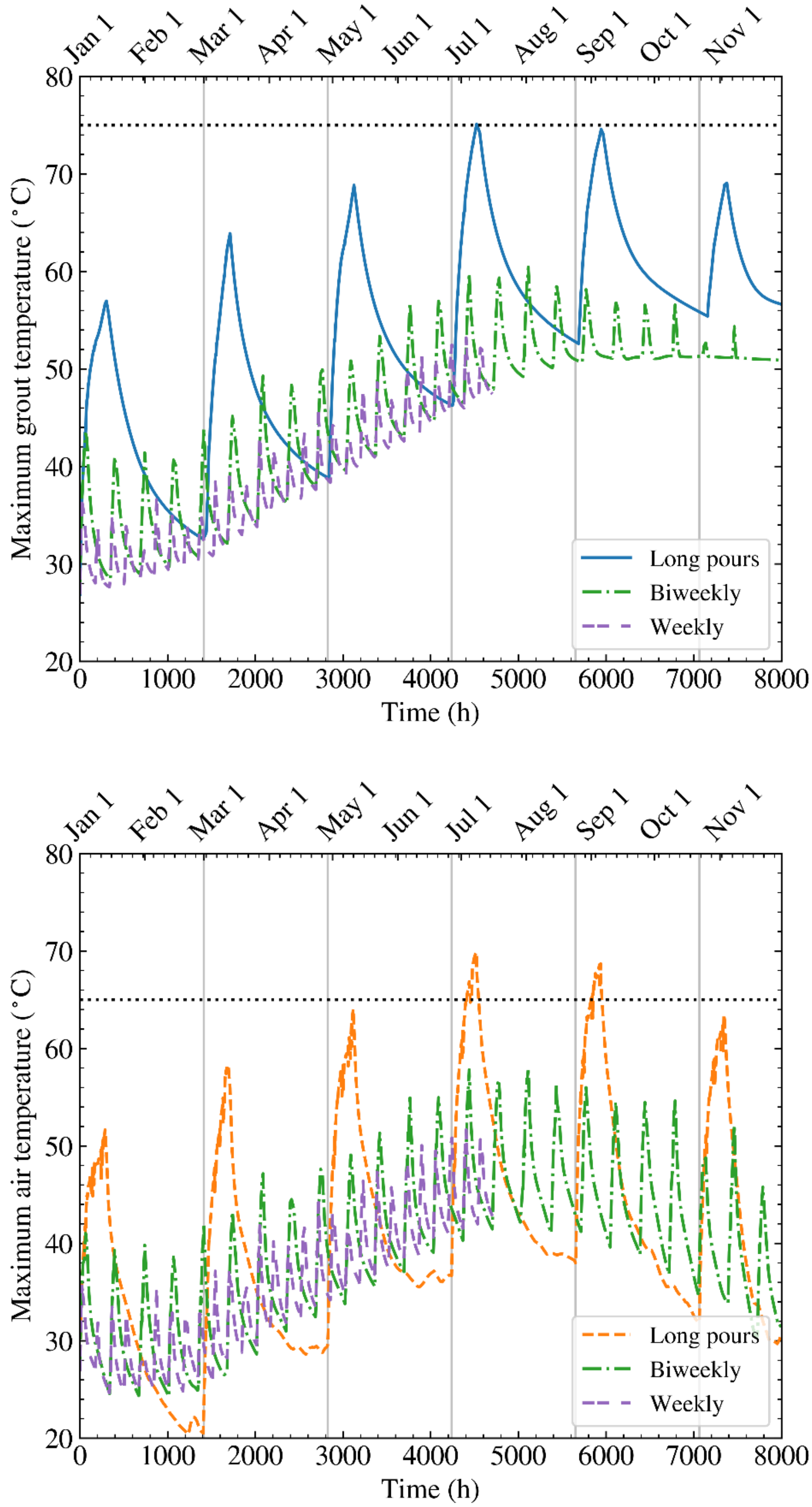

Figure 6. Comparison of maximum grout (upper) and air (lower) temperatures predicted for different pour schedules (long pours: 12.3 days pouring + 46.6 days idling; biweekly: 70.35 h + 265.65 h [nominal]; weekly: 35.17 h + 132.83 h [nominal]). The vertical gray lines indicate the starts of the pours in the long-pour schedule. The horizontal dotted lines indicate the relevant DSA limits.

Time interval (h)	Maximum grout temperature (°C)		
	Long pours	Biweekly	Weekly
0 – 1413	57.0	43.1 (−13.9)	36.6 (−20.4)
1413 – 2826	63.9	49.9 (−14.0)	45.6 (-18.3)
2826 – 4239	68.8	56.9 (−11.9)	52.5 (−16.3)
4239 – 5652	75.1	60.4 (-14.7)	–
5652 – 7075	74.6	58.1 (−16.5)	–

Table 3. Comparison of maximum grout temperatures for the different pour schedules, within time intervals bound by the starts of the long pours. The numbers in parentheses indicate the differences from the corresponding long-pour values.

Discussion

The SDU 6 model investigated here covers approximately one year of operations, during which the SDU is approximately half-filled with grout. For the long-pour schedule, the peak temperature expected in the second year of grout pouring can be estimated as follows (assuming the current DSA restriction on the grout height is lifted). For the run starting in January, the peak temperatures at the end of the seventh pour are 7 °C higher than those at the end of the first pour (Table 2). A sensitivity analysis found that a 1 °C increase in the ambient temperature led to a 0.8 °C increase in the maximum grout temperature [1]. As the average ambient temperature was 4 °C higher during the seventh pour, approximately half of the temperature difference between the seventh and first peaks can be attributed to the ambient conditions, and approximately half to the underlying layers of warm grout. Therefore, neglecting differences in the ambient conditions, the second year of operations will be starting from a peak temperature a few degrees higher than the peak at the start of the first. It is therefore reasonable to assume that the peak temperatures during the second year will be ~5 °C higher than the corresponding peaks during the first year. Hence, the 10th and 11th pours (starting in June and August, respectively), would likely result in peak grout and air temperatures of ~80 and ~75 °C, respectively. However, the precise values will be sensitive to the ambient conditions during that second summer.

A similar line of argument applied to the run starting in July leads to a similar estimate, though in that case the maximum temperatures would be expected at the end of the 13th and final pour. There is insufficient information to make a corresponding estimate for the shorter-duration pours. However, the temperatures in the second year are unlikely to be more than ~5 °C higher than in the first year, as the underlying grout is cooler than in the long-pour case.

The predicted maximum temperatures for the long-pour schedule exceed the limits in the DSA [3]. However, the model is known to be conservative: due to the lack of convection in the vapor space, the model tends to overpredict the temperatures. During benchmarking against data from SDU 2A with similar time-step and convergence criteria to those used here, the model overpredicted the peak grout temperature by about 10 °C [2]. In addition, the modeled pour schedule is very aggressive. Pouring on a biweekly schedule (with the same annual grout pouring rate) results in maximum temperatures that are about 10–15 °C lower than the long-pour schedule, and within the DSA limits.

Conclusion

One year of filling SDU 6 with cement-free grout has been simulated using an ANSYS Fluent model developed at SRNL [1] and currently owned by SRR [2]. Several different pour schedules were investigated [4].

The primary pour schedule investigated consists of seven 12.3-day pours separated by 46.6-day idle periods, resulting in 22.5 feet of grout being poured. For a run starting on January 1st, the maximum temperatures occur at the end of the fourth pour, in July. The maximum grout and air temperatures are 75.1 and 69.9 °C, respectively. For a run starting on July 1st, the maximum temperatures occur at the end of the seventh pour, in June. The maximum grout and air temperatures are 76.1 and 70.9 °C, respectively. It is estimated that the maximum temperatures during the second year would be about 5 °C higher. These temperatures exceed the limits in the DSA [3]. However, the lack of convection in the SDU vapor space means that the model tends to overpredict temperatures.

A less aggressive, biweekly pour schedule (70.35 h pouring + 265.65 h idling [nominal]) results in lower temperatures while maintaining the same average annual grout pouring rate. The predicted maximum grout and air temperatures are 60.4 and 58.0 °C, respectively, which are within the DSA limits. These occur around August 1st (for a run starting on January 1st). A weekly pour schedule (35.17 h pouring + 132.83 h idling [nominal]) predicts temperatures a few degrees lower than the biweekly pour schedule.

References

1. Lee, S. Y., *Thermal Analysis of Saltstone Disposal Units*, SRNL-STI-2019-00015 (Rev. 0), February 2019.
2. Henley, D. B., *Automating and Increasing the Speed of the ANSYS® Fluent® SDU Thermal Model*, G-ESR-Z-00028 (Rev. 0), 28 February 2019.
3. *Saltstone Facility Documented Safety Analysis*, WSRC-SA-2003-00001 (Rev. 15), July 2018.
4. Brooks, T. and S. Simner, *SDU Thermal Model Inputs*, SRR-SDU-2016-00021 (Rev. 2), 14 November 2016.
5. *Z Area Saltstone Disposal Site SDU6 Tank Design Concrete Wall and Column Section and Details*, C-CC-Z-00042 Sheet 0 (Rev. 10), 19 Jan 2017.
6. Chew, D. P., B. A. Hamm, and M. N. Wells, *Liquid Waste System Plan*, SRR-LWP-2009-00001 (Rev. 21), 31 January 2019.
7. Mangold, J. E., *Recommended Input Values for Thermal Model Development*, SRR-CWDA-2018-00074 (Rev. 0), 18 October 2018.
8. Press, W. H., S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C: The Art of Scientific Computing*. 2nd ed., Cambridge: Cambridge University Press, 1992. Available from: http://apps.nrbook.com/c/index.html.
9. *scipy.optimize.brentq*. 5 May 2018 [accessed: 23 October 2018]; Available from: http://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.brentq.html.

APPENDIX: CALCULATING THE AMBIENT TEMPERATURE FROM THE FLUENT OUTPUT

Given F and T_S from the Fluent output, Equation (1) can be solved for the ambient temperature, T_{amb}. However, because the equation is fourth-order in T_{amb}, there will be up to four independent solutions. Care must therefore be taken that the correct, physical solution is found.

To determine the nature of the solutions, begin by rewriting Equation (1) as

$$y(T_{\text{amb}}) \equiv \sigma\epsilon T_{\text{amb}}^4 + hT_{\text{amb}} + F - hT_s - \sigma\epsilon T_s^4 = 0 \tag{2}$$

and differentiating with respect to T_{amb}:

$$\frac{dy}{dT_{\text{amb}}} = 4\sigma\epsilon T_{\text{amb}}^3 + h. \tag{3}$$

This implies that the only stationary point ($dy/dT_{\text{amb}} = 0$) is at $T_{\text{amb}} = -(h/4\sigma\epsilon)^{1/3}$. Since $y \to +\infty$ as $T_{\text{amb}} \to \pm\infty$, this stationary point must be a minimum.[3] Now, since there must at least one solution to Equation (2) with $T_{\text{amb}} > 0$ (i.e., the physical solution), the constant $F - hT_s - \sigma\epsilon T_s^4$ in the equation must be negative, and hence $y(T_{\text{amb}} = 0) < 0$. Therefore, since $y \to +\infty$ as $T_{\text{amb}} \to \pm\infty$, $y(0) < 0$, and $y(T_{\text{amb}})$ has exactly one stationary point (a minimum), it follows that Equation (2) has exactly two real solutions for T_{amb}, only one of which is positive (and therefore physical; see Figure 7).

In practice, Equation (2) was solved numerically for T_{amb} using Brent's method [8, §9.3], as implemented in the Python SciPy package [9]. This method is guaranteed to converge if the initial interval contains the solution. Therefore, for each time in the model a solution was sought between 0 K and a temperature known to be higher than the actual ambient temperatures (400 K), thus guaranteeing that the solver found the desired physical solution to Equation (2).

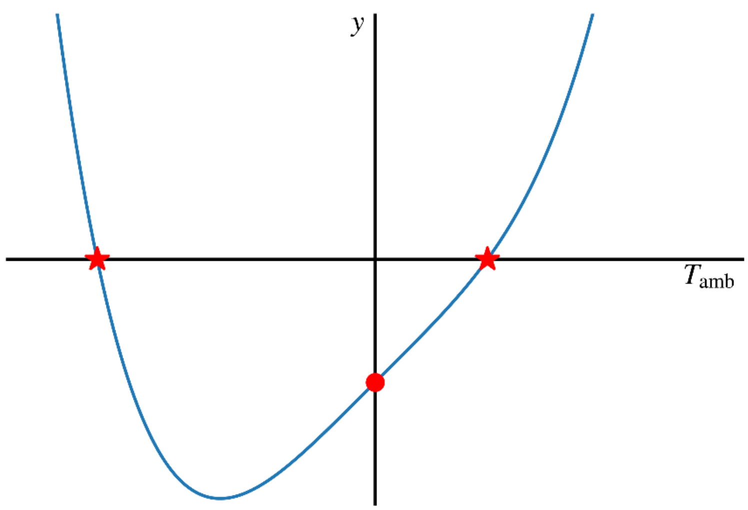

Figure 7. Illustration of the curve $y(T_{\text{amb}})$ given by Equation (2). Since $y \to +\infty$ as $T_{\text{amb}} \to \pm\infty$, $y(0) < 0$ (red circle), and $y(T_{\text{amb}})$ has exactly one stationary point (a minimum), it follows that $y(T_{\text{amb}}) = 0$ has exactly two real solutions (red stars), only one of which is positive.

[3] This is confirmed by considering the second derivative: $d^2y/dT_{\text{amb}}^2 = 12\sigma T_{\text{amb}}^2 > 0$ for all T_{amb}.