Analysis of Sensitivity of VCCTL Measurements to Various Input Quantities

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Abstract

Virtual measurements are the outputs of well-defined mathematical models based on theoretical principles and simulation algorithms. The VCCTL (Virtual Cement and Concrete Testing Laboratory) is a software system built by the Materials and Construction Research Division of NIST to perform computations of various physical properties of portland cement-based materials. Its intended use is as a research/exploratory tool to model the formation of concrete, which is a complex random material, over length scales ranging from nanometers to millimeters.

This article describes our efforts at exploring the use of random numbers in the VCCTL software to mimic the randomness encountered in real concrete systems. We have examined the effects of the choice of random number seeds for a random number generator used in the cement hydration simulations. Further, we have performed preliminary sensitivity analysis of the VCCTL measurements to changes in the time conversion parameter, β, and changes in the way that random correlation functions are used in describing cement particle structure. For a particular subset of portland cements, there are accurate physical measurements obtained by large inter-laboratory experiments coordinated by the Cement and Concrete Reference Laboratory (CCRL). We used this data as a measure of the accuracy of the VCCTL predictions and as a way to compute one parameter needed in the VCCTL simulations, the β parameter.
Keywords: Sensitivity analysis, virtual measurements, computer experiments

1. Introduction

The VCCTL system predicts measurements of physical properties of many types of cement-based materials. Physically, one selects a cement powder to mix with water. The cement reacts with water in an exothermic reaction, releasing heat that can be measured. The reacted cement powder plus water is called cement paste. Cement paste forms the matrix phase for composite materials like mortar (cement plus sand plus water) and concrete (cement plus sand plus gravel plus water). The cement powder comes in a range of particle sizes, from about 0.5 μm to about 30 μm. The shape of the particles, itself a random variable, is similar to the shape of crushed gravel, and can display aspect ratios of up to 3:1. This aspect of randomness is ignored in this paper and the particles are modeled as spheres. Each particle is made up of one or more chemically distinct phases, all which react differently with water, and which can occur randomly in the particles.

In the VCCTL package, the location of each cement particle in the mixture is a random variable, the distribution of different chemical phases in each particle is a random variable, and the various reactions with water are modeled as stochastic processes. The modeling process can be summarized as follows. First, a model microstructure of a particular cement, a 3-D cube, is created as a lattice with randomly placed digitized spherical cement particles with a specified size distribution. Second, the main chemical phases are distributed over the cement particles. This step uses measurements of the amounts of the chemical phases as measured by a scanning electron microscope (SEM) image of a sample of the actual cement. The actual amounts of the phases in the particles, on average, as well as two-point correlation functions that approximately describe how these phases are distributed among the particles, are measured with the SEM and are approximately and randomly matched in the model microstructure.

After these steps, the digital microstructure is subjected to hydration, i.e., a chemical reaction between cement chemical phases and water. This is modeled by a cellular automaton process that simulates hardening of the cement by dissolving portions of the boundary of each particle and letting the dissolved voxels perform random walks until they meet other dissolved voxels. Two voxels that meet can nucleate and form a new particle of reaction product and reduce the void space. This algorithm is repeated in cycles. The VCCTL gives results in terms of number of cycles run. The heat released can be easily computed since it is known in the model how much of each phase has reacted, and the heat released for each kind of reaction is known. Cycles are then related to elapsed time (hours) by a transformation, i.e., time is the squared number of cycles multiplied by a conversion factor (β). This produces one of the virtual measurements, that is, the heat of hydration (HH) measurement. After hydration, separate modules of the program compute other measurements such as elastic moduli, electrical conductivity, and compressive strength. These virtual measurements will not be further discussed in this paper, but attention will be paid only to the heat of hydration measurements. Further information on this system can be found in Bullard(2004).

We chose to study several important features of the VCCTL in this paper in regards to how randomness is simulated. First, there are three random seeds used in the creation of cement paste microstructure and their effect on the virtual measurements was of interest. In particular, we wanted to see their effect on the non-random β conversion factor from cycles to time, since this parameter is important when comparisons to real physical measurements are to be made.

2. The effects of choice of random seed on heat of hydration

As was discussed in the introduction, the VCCTL software requires the user to input three random seeds. The first is used in the creation of the initial 3-D microstructure to essentially randomize where the particle placement sites are located. The second random number seed is used to give a random start in the distribution of the clinker chemical phases amongst the cement particles. The third random seed is used in the hydration module, to give this process a random start. It was of interest to determine how much of an effect the choice of seed has on the output of the VCCTL. This determination had never been systematically carried out before. A given run was made with values chosen for all three random seeds. A plot of heat released vs. number of cycles was made. This is converted to a heat released vs. elapsed time plot via the using the equation time = β (# cycles)^2. The CCRL database has measured heat of hydration values, with uncertainties computed over many laboratories, for the cement paste at 7 days and 28 days. Changing the value of β only moves the model data points left or right along the time axis, so the optimal value of β is chosen by a least-squares fitting to the two known data points of heat of hydration (heat released during hydration) at the two known times. Then the heat released at 7 days and 28 days (in kJ normalized by the mass of cement used in kg) from the VCCTL simulation run can be interpolated from the virtual data and compared to the experimental results.

Table 1 summarizes VCCTL predictions of heat of hydration for CCRL cement 152. Thirty-three different sets of random number seed values were chosen and an equivalent run was made using each set. Each set of values was called a different "treatment." Taking the 33 runs as simple replicates, we obtained standard deviation of 0.91 kJ/kg for the 7 day heat of hydration and 2.27 kJ/kg for the 28 day heat of hydration. This gives a relative standard deviation of 0.25 % for the 7 day heat of hydration VCCTL measurements, when sampled with different random seeds. For comparison, the relative standard deviation of the CCRL experimental measurements for the 7 day heat of hydration of cement 152 was 8.45 %.

	7-day HH (kJ/kg cement)	**28-day HH** (kJ/kg cement)
VCCTL Mean	364.66	417.91
VCCTL std	0.91	2.27
CCRL Mean	367.28	412.42

Table 1. Summary statistics for heat of hydration for all random seed runs.

Analysis of variance (fixed effects model) was used to determine whether the choice of any of the three random seeds had any effect on the measurements of 7 day and 28 day heat of hydration. It showed that there was no such effect.

It is also of interest to determine whether random seed choice had any effect on the difference between the VCCTL value and the corresponding CCRL value. A subset of our data set formed a full 2^3 factorial experiment with factor 1 = seed 1, factor 2 = seed 2, and factor 3 = seed 3. The levels of each factor were: level 1 = -8118 and level 2 = -2222. A formal analysis of variance of the 7 day bias terms showed no effect of any of the three factors, that is, there was no difference between the bias at level 1 of factor *i* and the bias at level 2 of the same factor. For the 28 day bias, there was a significant effect of the 1st seed.

	Df	**Sum Sq**	**Mean Sq**	**F**	**Pr(F)**
Seed 1	1	7.61	7.613	14.788	0.0184
Seed 2	1	1.80	1.799	3.494	0.135
Seed 3	1	0.22	0.217	0.421	0.552
Resid.	4	2.06	0.518		

Table 2. Results of an analysis of variance for the simulation data that formed a full 2^3 factorial experiment.

Further analysis shows that the 28 day bias is larger for seed 1 = -8118 than for seed 1 = -2222. The largest average bias is 6.7 kJ/kg, so the relative bias is 1.6 %. The largest relative standard deviation is 0.63 % for seed1 = -32767. For comparison, the relative standard deviation of the CCRL experimental measurements of the 28 day heat of hydration f cement 152 is 5.83 %.

To summarize this section, for cement 152, the choice of random number seed has a relatively minor effect on the difference between the VCCTL numerical value and the corresponding CCRL experimental value. In particular, the choice of the 1st seed, the one that gives a random start to the particle placement algorithm, has some effect on the 28 day bias. The relative standard deviations of the VCCTL measurements computed over the data sets with various random seeds are about one tenth of the relative standard deviations of the corresponding CCRL data.

3. Influence of single run β vs. using the average β

The β parameter is used to convert cycles to time, enabling a comparison of VCCTL predictions to CCRL measurements. The value of β was computed for each run, for each choice of the random number seeds, using a least-squares algorithm that minimizes the distance between the VCCTL measurement and the corresponding CCRL measurement. In the future, when the VCCTL is used to predict properties for cements not in the CCRL, it would be useful to know if a default β parameter could be used for different random number seeds, mixture proportions of cement and water, type of cement, and other parameters. As an alternative, β can be determined from an early-age (1 day) measurement of a physical property such as chemical shrinkage, see Bentz(2007). In this paper, we only examined the effect of random number seed choice on the value of the β parameter.

To examine the effect of β on the accuracy of the VCCTL measurements, when the values of the random number seeds were varied, fifteen different runs (with different random seeds) were used to compute the heat of hydration for cement 152. For each run, the optimal β was computed and used to obtain the measurements. In addition, an average β was computed for the 15 runs (0.00044 h/cycles^2) and then each run was repeated using the average β. The resulting data form a set of 15 heat of hydration values for the optimal β and 15 for the average β. Table 3 summarizes the data. It shows that the differences between the optimal and average β derived heat of hydration values are somewhat larger for the 3 day and 7 day heat of hydration than for the 28 day heat of hydration. It also shows that the standard deviation of the runs is larger if the average β is used than if the optimal β is used. This is especially true for the shorter hydration runs, i.e., 3 day and 7 day. It is also sensible that the earlier times are associated with the greater variations, because, physically, the rate of heat evolution with time is much greater at earlier times than at later ages. Thus it appears that using only a single value of β without regards to the choice of random number seed for a given cement could possibly be used but would be more accurate for the longer duration hydration runs.

HH (kJ/kg)	**3 d opt**	**3 d avg**
Mean	307.97	308.24
Std	1.17	5.77
	7 d opt	**7 d avg**
Mean	364.87	365.10
Std	1.43	5.01
	28 d opt	**28 d avg**
Mean	418.47	418.63
Std	3.03	4.05

Table 3. Summary statistics for average (avg, 0.00044 h/cycles^2) and optimal (opt) β runs for various random seeds.

4. Conclusions

Our main conclusions are as follows. First, the results obtained from the VCCTL software have variation or randomness in results due to different random number seeds that equals approximately one tenth of the measured CCRL variation. That means that for the purpose of producing predictions that agree with experimental measurements within experimental uncertainty, one can ignore the random number seed values. This is an interesting result, and will have an impact on the future structure and operating instructions for the VCCTL. Second, for a particular choice of cement, cement 152, it seems that for longer duration (28 day) hydration runs a default value of β specific for a given cement performs very well, and reasonably well for the 7 day results. Again, this is probably due to fact that in the actual physical situation, the rate of heat production or reaction is much more in the earlier ages than in the later ages.

References

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