Monte Carlo simulation and evaluation of burst strength of pressure vessels

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Article Information

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The Monte Carlo method enables the statistical simulation of the mechanical properties of groups taken from a given population. In the case of composite pressure vessels used for hydrogen storage, properties like burst strength or fatigue cycle strength are of interest. This paper provides comprehensive information on how populations are generated and how samples can be taken and evaluated; it also explains how to determine the acceptance rate of random samples from simulated populations for passing the approval test "minimum burst pressure". A word of caution is also expressed regarding the evaluation of acceptance rates from a small sample.

For over 10 years, the Federal Institute for Materials Research and Testing (BAM) has been developing and improving statistical methods for the probabilistic approach (PA) to assess the safety of composite compressed gas storage systems [1], particularly with respect to their use for the storage of hydrogen. The PA developed [2-6] is based on sample testing and statistical assessment in combination with reliability criteria. Monte Carlo simulation (MCS) [7, 8, 9] plays a significant role in simulating the mechanical properties of composite pressure vessels (CPV) such as burst strength [10, 11] or fatigue strength [12]. In the meantime, the acceptance rate of a product population according to different acceptance criteria can be determined as well. Through MCS the minimum requirements for standards and regulations are examined and the potential for improvement is elaborated [13].

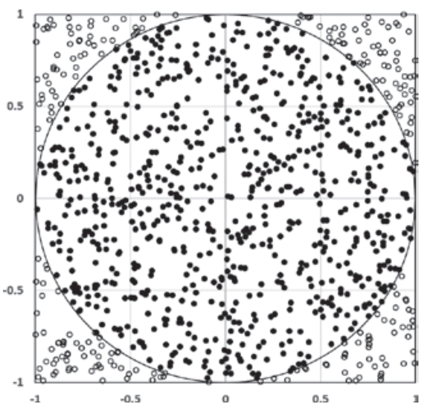

Figure 1: Approximation of pi via Monte Carlo simulation

MCS is based on statistics and probability theory. To understand the results of these simulations, it is necessary to explain the approach step by step via a simple and comprehensible example.

The principle of MCS can be demonstrated by a simple experiment for approximating the value of the number π ("pi"). Figure 1 illustrates a unit square with an enclosed unit circle. The points in the diagram are generated by MCS in a random and independent manner. The number of points generated in the unit circle (P_C) in relation to the number of points in the unit square (P_S), will be close to the ratio of the corresponding areas A_C and A_S if the number of points is sufficiently large:

$$\frac{P_C}{P_S} \approx \frac{A_C}{A_S} = \frac{\pi\, r^2}{(2r)^2} = \frac{\pi}{4} = 0.78540 \qquad (1)$$

As a simple and clear illustration, only 1000 points are shown in Figure 1. The result of this experiment is listed in Table 1 to show the convergence of the approximation of π (pi) depending on the number of points generated by the MCS.

The results in Table 1, based on the exemplary points shown in Figure 1, visualize how a good approximation to the number π can be achieved statistically through experiments in MCS by a random and independent arrangement of points. In addition, it can be shown that the higher the number of generated points, the better the approximation. The results from this series of simulations gradually converge to an accurate solution of pi.

Example of Monte Carlo simulation

MCS is based on random numbers and thus on the application of a random number generator. As an example of a possible procedure for a normal distributed MCS, the polar method is presented below.

Polar method. The random MCS numbers are generated by a random number generator which is usually embedded in numeric software. As an example of normal distributed data generated by MSC, the polar method is explained below.

The polar method developed by Marsagalia and Bray [14] is one of the possible methods to generate normal distributed random data. It serves as a random number generator for the required primitive data in a MCS. The polar method hearkens back to the Box-Muller algorithm for generating normal distributed random variables by using Euclidean coordinates. In the polar method random points in the plane are produced and are arranged approximately uniformly in an imaginary unit circle with radius r = 1. The coordinates for the points are generated from random numbers.

Generating random number according to Figure 2

Step 1: In the polar method, according to section 5.2.1 in [1], two random numbers, Z_1, Z_2, for each simulated individual are generated independently by means of a random number generator in an interval of [0 ... 1]. The data thus created are depicted as dots in Figure 3.

Step 2: In the next step, the values of the coordinates in the unit circle u and v from the previously pairwise generated random numbers are determined according to the following equations:

$$u = 2 \cdot Z_1 - 1 \tag{2}$$

$$v = 2 \cdot Z_2 - 1 \tag{3}$$

In Step 3, values of the auxiliary quantity q for each individual i are calculated:

$$q_i = u^2 + v^2 \tag{4}$$

Total number of points P_Q within square	Number of points P_K within circle	P_K/P_Q acc. to Equation (1)	Approximation of figure π: $4\,(P_K/P_Q)$
10	9	0.9000	3.6000
100	87	0.8700	3.4800
1,000	806	0.80600	3.2240
4,000	3,195	0.79875	3.1950
10,000	7,899	0.78990	3.1596
50,000	39,269	0.78538	3.1415

Table 1: Approaching the value of the number pi by increasing the total number of random points

If numerical values for q are obtained, for which q = r > 1, these individuals must be excluded. The results for qi are shown in Figure 3.

In Step 4, values for the deviation measure x of the normal distribution are calculated:

$$x_i = u \cdot \sqrt{\frac{-2 \cdot \ln q_i}{q_i}} \tag{5}$$

This yields the data shown in Figure 4. Each point represents an individual or a property of an individual considered. The total set of points shows the entire generated population of individuals.

By applying the condition in Step 3, the numerical data of q, corresponding to the individuals i are excluded if they are outside the unit circle (q = r > 1). Unless replacement data are regenerated, the number of simulated individuals in the further calculation of the polar method decreases accordingly.

Apart from using the polar method to generate the normal distributed properties of individuals, the "inverse function" of the normal distribution of customary programs can also be used in combination with a random number generator. Figure 4 shows an example of a data cloud generated with Microsoft Excel (2016 MSO – Version 1803).

Generating the population. In the following, the random numbers generated are used to simulate the burst strength property of a population of CPVs (composite pressure

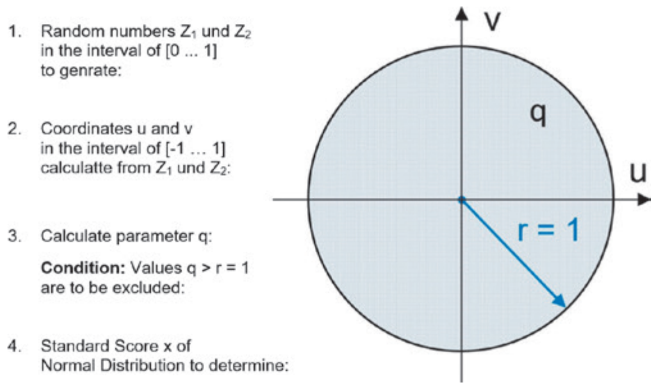

Figure 2: Overview of calculation steps of polar method based on the unit circle with the radius r = 1

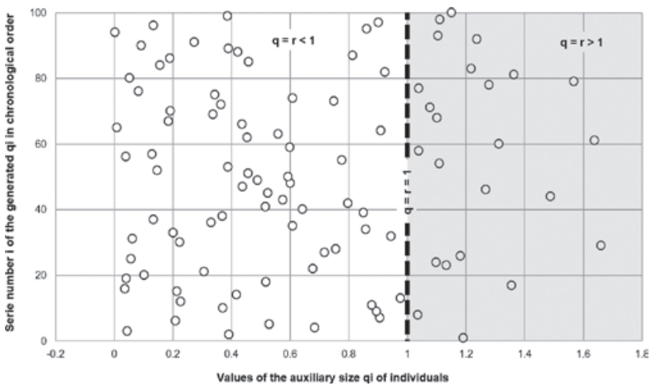

Figure 3: Polar method Step 3: sorting the parameter q_i calculated from a pair of random number Z_{1i}, Z_{2i}

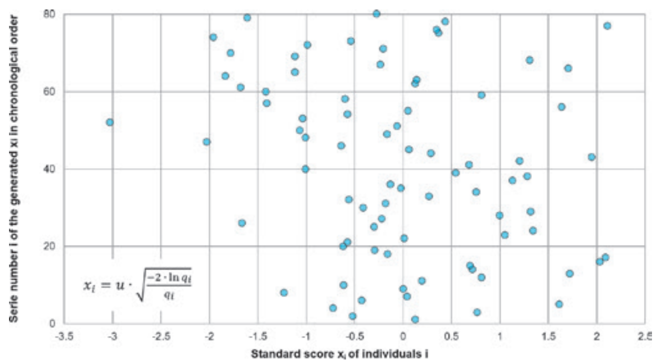

Figure 4: Polar method Step 4: cloud of individuals with standard score x_i

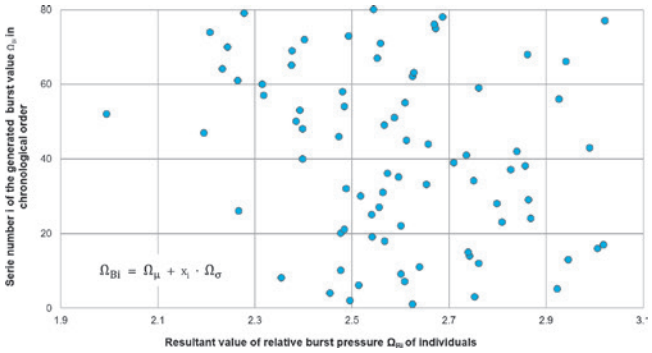

Figure 5: Polar method Step 5: relative burst pressure Ω_{Bi} of individuals for a population of 80 individuals

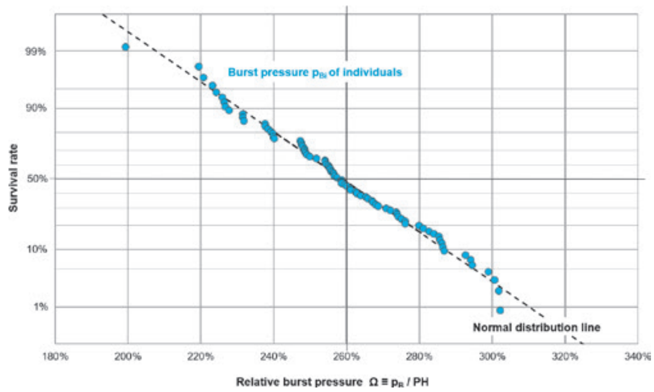

Figure 6: Monte Carlo simulation of a normal distributed population sorted in a Gaussian probability net

vessels) used for storing hydrogen in vehicles as a propellant or for transport.

The properties of a population are described in Figure 5 by the two normalized parameters of the burst strengths test results simulated by MCS: "mean strength Ω_μ" and "standard deviation Ω_σ". The determination of the basic values Ω_μ and Ω_σ is necessary as the essential input for the basic population; to be combined with the standard score x_i for generating properties of the population. More specifically, these central characteristics Ω of the total population as well as the properties of samples used comparatively below are normalized to a maximum service pressure (MSP). By means of normalization, the relative burst strength and relative standard deviation are obtained, which can be used in a specially prepared, standardized working diagram.

In order to obtain the burst strength Ω_{Bi} of an individual i, the generated standard score x_i of an individual is combined with the defined properties of the total population [6]:

$$\Omega_{Bi} = \Omega_\mu + x_i \cdot \Omega_\sigma \tag{6}$$

The example used in the following is based on "mean" and "standard deviation" determined as:

Ω_μ = 2.6 for mean burst pressure
Ω_σ = 0.2 for standard deviation.

Verification of the statistical distribution. Often, it is necessary to check, whether the expected distribution (here Gaussian normal distribution) is actually generated [16].

Pressure vessels are designed and manufactured for a guaranteed minimum burst pressure. In fact, the real strength of burst pressure mainly varies due to material and manufacture reproducibility, so that it can never be statistically ruled out that the guaranteed minimum burst value of a few individuals may be lower than the accepted minimum requirement.

The Gaussian probability net (see section 3.2.1 from [1] and [17]), is often applied to check the normal distribution function for the data of Ω_{Bi}.

Figure 6 shows a comparison between the strength data (points) generated and an ideal normal distribution (straight line) in a Gaussian probability net. Since all data scatter closely around the straight line, there is no indication that the values generated are not distributed normally. The dashed line in Figure 6 represents the theoretical normal distribution. The gradient of the best fit or regression line describes the standard deviation of the normalized burst pressure of the population generated. An increase in the gradient of the best fit line indicates a reduction in standard deviation.

Generating the samples. To simulate the real scenario of compiling a sample, the CPVs must be drawn from a population. This can even be simulated via MCS. For this purpose, each randomly generated CPV is simulated as if "pulled" from the population. Each sample is collected according to the given sample size, i. e. number of elements n in the sample, e. g. n = 3, 5, 7, and then statistically evaluated. The sequence of "pulling single CPVs from population" can be done randomly or subsequently depending on the requirements of a real scenario. The process is shown in Figure 7 for the sample data selected with an extreme sample size of n = 3. The three individual values of the randomly selected CPV are each shown in Figure 7.

The number n of CPVs in a sample influences the deviation of a sample from the Ω_μ and Ω_σ determined. The larger the sample size, the less a sample usually deviates from its true value. This means that the more the area is narrowed down, the more confidently the results of the statistical assessment can be achieved (see section 3.4.1 from [1]). The absolute minimum of a sample size is n = 3 and is used as the simplest example in the following to demonstrate the principles of MCS.

Evaluating the samples. In the next step, a classical acceptance criterion is added to the evaluation. For the relative burst pressure of each individual, a minimum strength value of 2.3 times the maximum service pressure (MSP) is required. This corresponds to a minimum value of twice the test pressure for pressure receptacles according to [15] as long as the maximum service pressure, which is here the gas pressure at 65 °C, does not exceed 85 % of the test pressure, as described for exam-

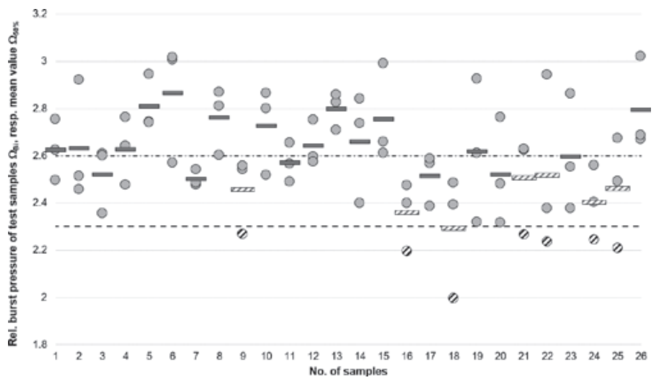

Figure 7: Deterministic evaluation of the samples according to a minimum value of requirement

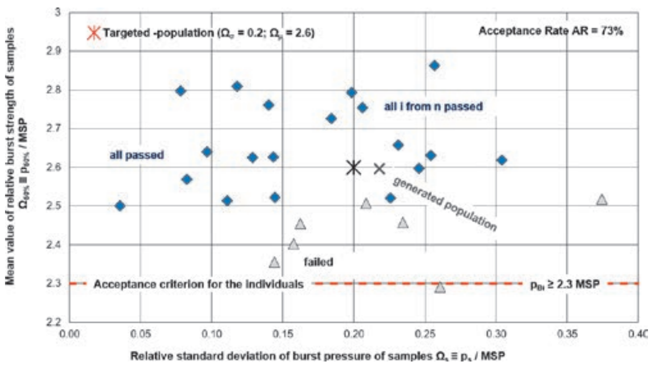

Figure 8: Monte Carlo simulation of sample property "burst" in a SPC, population of 80 individuals, sample size n = 3 and number of samples 26

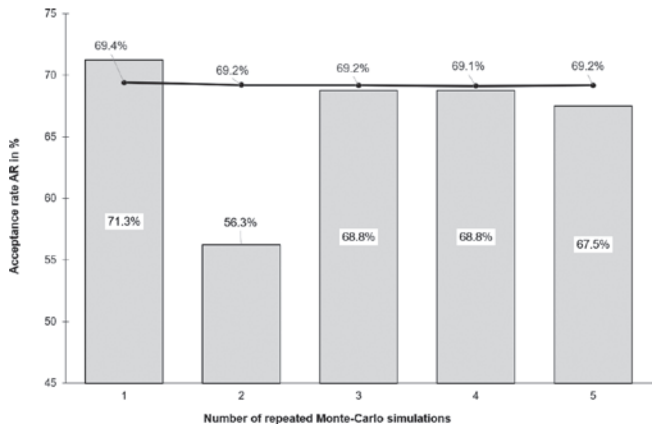

Figure 9: Discrepancies of acceptance rate depending on number of samples, bar graph (sample = 26), line graph (sample = 16,666)a

ple for hydrogen. All individual strength values that meet the minimum requirement are shown as a grey spot in Figure 7 (passed); individual values below the minimum value are indicated as a hatched spot (failed). Each of these individuals has been randomised as a part of a sample. The associated mean values of each sample are indicated as a horizontal bar following a comparable indication system. The overall targeted average of 2.6 is added. In this way, the acceptance criteria for the burst test of different sets of rules can also be considered [11].

Figure 8 shows these results of sample testing in the sample performance chart (SPC) introduced in Section 3.1 from a previous publication [1] to demonstrate the quality of "burst strength". The mean and standard deviation of the respective sample are calculated from the burst strength values of each of the 3 individual CPVs per sample. Thus, the sample properties simulated are represented by means of one mark in the diagram. Hence, from a total of 80 individuals generated, 26 random samples of 3 individuals are evaluated.

If all individuals of a sample meet this deterministic minimum value, according to Figure 7, each mark representing the entire sample in Figure 8 is indicated as a diamond. If the sample contains one or more individuals that do not meet the minimum strength requirement, the sample is shown as a triangle. These failed samples have a relatively lower mean strength and exhibit a higher standard deviation.

The acceptance rate is obtained if the ratio of the number of blue dots (22 samples) in relation to the total number of samples (26) is calculated. The acceptance rate AR for the population simulated and exemplarily evaluated here ($\Omega_\sigma = 0.2$, $\Omega_\mu = 2.6$) is AR = 85 %. As shown in [1, 11, 12], the effects of different acceptance criteria in terms of burst strength [8] and load cycle strength [12] according to various standards and regulations for the approval of CPVs have been presented.

Small sample effect on acceptance rate. The example demonstrated in this paper is based on a small number of samples (26) and an extremely small sample size (n = 3). It it clear that the use of a small number of samples for calculating the acceptance rate is a flaw, causing discrepancies in the acceptance rate due to repeated identical MCSs.

The acceptance rates presented in Figure 9 as a bar graph are obtained from MCSs which were run five times separately with identical parameters. The acceptance rates vary from the lowest 56.3 % to the highest 71.3 % by evaluating 26 samples (78 CPVs for n = 3) with an assumed acceptance criterion of 250 % MSP. A maximum of 15 % deviation from the acceptance rate results of the simulations repeated five times using a small number of samples. This effect is less significant if the number of samples increases. The line in Figure 9 shows a maximum difference of 1 % if the number of samples increases to 16,666 (about 50,000 CPV for n = 3).

Obviously the discrepancy in the acceptance rate in the MCS depends on the number of samples and the amount of elements per sample or the total number of selected CPVs when conducting a statistical assessment. A convergence study of the discrepancies in the acceptance rate depending on the number of samples has not been carried out here. However, a word of caution is expressed with respect to using samples to simulate and evaluate the effectiveness of standards and regulations. It is important to check the quality of a series of manufactured pressure vessels even with a small number of small samples rather than based on the results of a single test.

Conclusions

The Monte Carlo simulation is a suitable method for obtaining strength properties such as burst strength and fatigue strength of composite pressure vessels. The simulation of pressure vessel populations and samples taken from these basic populations allows for an evaluation of the effectiveness of minimum requirements that would otherwise not be possible because of the extreme effort to carry them out. This in turn enables a systematic analysis of the way of taking effect of deterministic minimum requirements and the improvement of appropriate approval requirements. However, there is a particular effect of small samples which must be taken into account when evaluating test data.

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