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Convergence Analysis of a Markov Chain Monte Carlo Based Mix Design Optimization for High Compressive Strength Pervious Concrete

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Abstract. Compared with conventional concrete products, pervious concrete usually features with high water permeability rate and low compressive strength due to the lack of fine aggregates. Thus the determination of optimal mix design of ingredients has been recognized as an effective mechanism to achieve the trade-off between compressive strength and permeability rate. In this paper, we proposed a Markov Chain Monte Carlo based approach to approximate the optimal mix design of pervious concrete to achieve a relatively high compressive strength while maintaining desired permeability rate. It is proved that the proposed approach effectively converges to the optimal solutions and the convergence rate and accuracy rely on a control parameter used in the proposed algorithm. A number of simulations are carried out and the results show that the proposed system converges to the optimal solutions quickly and the derived optimal mix design.

1. Introduction

Pervious concrete is formed by mixing cement, water and coarse aggregates [1]. Due to the excellent permeability of pervious concrete, it has been widely used in urban construction and pavement. The component of cement paste usually forms a thick layer of coating around the coarse aggregate, the small particles of coarse aggregate are strongly combined with the cement paste to enhance stability and provide the desired mechanical properties [1,2]. Due to the absence of fine aggregates, a large amount of vacancies between coarse aggregates can be observed inFigure 1. These vacancies result ina much higher permeability rate of pervious concrete compared with the conventional counterparts that is shown inFigure 2. Contrarily, the lack of fine aggregate weakens the pervious concrete on compressive strength. Therefore, an effective and efficient pervious concrete mix design optimization that achieves the maximum compressive strength while maintaining a suitable permeability rate to meet the construction requirement is desirable [1].

In this paper, a design of pervious concrete as a Markov Chain Monte Carlo (MCMC) process is modeled [2,3,4,5,6,7] and an optimization approach to approximate the optimal mix design based on Gibbs Sampling is proposed [2]. In order to achieve the aim of maximize the compressive strength while maintaining a relatively high permeability rate, the key problem of this paper is to find out an optimal mix design to obtain those features (i.e., optimal relative proportions of ingredients). As a result, a global optimal solution that effectively and efficiently converged by the proposed algorithm is discussed. The rate and accuracy of convergence is dominated by a control parameter employed in the approach. In addition, a number of simulations are carried out to implement the Makov Chain Monte Carlo based approach. From the simulation results, we could see that the

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system converges to the optimal mix design globally effectively and efficiently by using the Makov Chain Mnte Carlo based approach. Also the convergence of iteration is accurate and fast when the optimal system coefficients are used.

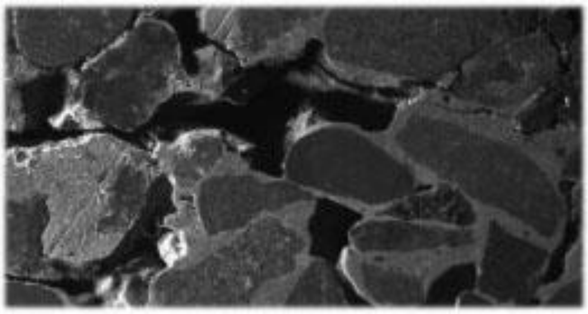

Figure 1. Material structure of pervious concrete.

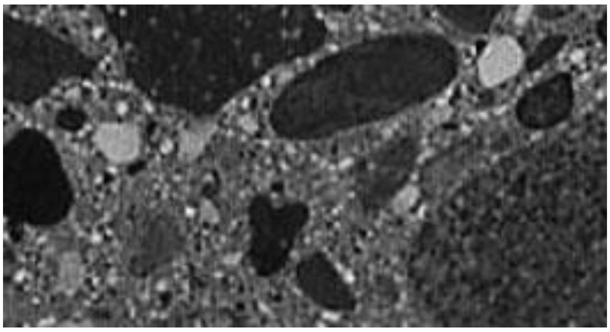

Figure 2. Material structure of conventional concrete.

The rest of this paper is organized as follows. In Section 2, the markov chain monte carlo technique and the Gibbs Sampling method are briefly reviewed. Section 3 describes a MCMC based pervious concrete model and a Gibbs Sampling method based optimization approach. The convergence analysis of the proposed algorithm is also depicted in Section 3. In Section 4, a number of simulations are carried out to show the effectiveness and efficiency of the proposed approach. Section 5 concludes this paper.

2. Methodology

The Markov Chain Monte Carlo (MCMC) technique is a general computing technique that has been widely used in physics and computer science, which include a family of algorithms for sampling from probability distributions based on constructing a Markov chain whose stationary distribution is the desired distribution. MCMC solve the complicated or high dimension problems by constructing a Markov chain having $\pi(\cdot)$ as its stationary distribution, and carry on the Monte Carlo method to the samples collected according to the $\pi(\cdot)$. Initially, the prior distribution may be arbitrary, the system transits its states randomly with small steps to generate and filter samples. Once the qualified samples are generated for the Markov chain, this chain will be executed for a relatively long time to reach its stable state, which is referred as burn-in process. Then, the stable samples will be used in the Monte Carlo integration to approximate the expectation of function.

The Gibbs Sampling method is one of the well-known MCMC sampling methods which carry out the Monte Carlo method to the samples collected from a stationary distribution π. In a given system, system variable vector x is a *N*-dimension row vector with element x_n, $n = 1, \cdots, N$ and the distribution of interest $F(x)$ is a function of vector x and can be of any form. The key idea of the Gibbs Sampling method is that the value of each random variable in the vector x is updated iteratively and asynchronously according to a probability distribution.

In each iteration, a sample is drawn from the conditional distribution $P(x_n \mid x_{-n}, F(x))$ where $x_{-n} = (x_1, \cdots, x_{n-1}, x_{n+1}, \cdots, x_N)$, $n \in [1, N]$. It can be seen that the Gibbs Sampling method defines a Markov Chain on variable x. Assuming $\chi = (\chi_1, \chi_2, \cdots, \chi_N)$ is the feasible real domain corresponding to random variable vector x, the detailed Gibbs Sampling method is given in Algorithm shown below.

Algorithm 1: Gibbs Sampling Algorithm

- Initialization: Randomly select an initial point $x \in \chi$;
- while $n \in N$ do
  - the element x_n is updated by a sample from the probability distribution $P_n(x_{-n}) = (P_n(x_n \mid x_{-n}), \forall x_n \in \chi_n)$ with

$$P_n(x_n \mid x_{-n}) = \frac{\exp(\frac{-b}{F(x_n, x_{-n})})}{\sum_{x_n' \in \chi_n} \exp(\frac{-b}{F(x_n', x_{-n})})} \qquad (1)$$

where b is a positive constant.
  - increment n by one;
  - if $n > N$, then $n = 1$;

According to (2), x_n which produces a higher value of objective function deserves a higher probability to be selected. In light of the Gibbs Sampling method, it becomes possible to estimate highly complicated models.
The weighted product method (WPM) is employed in our system to generate a utility function. WPM is one of the widely used multi-criteria decision making (MCDM) methods which allow one to carry out comprehensive analysis by taking account of multiple aspects of systems[1,2]. In a WPM system consisting of k system variables (e.g. $n_1, n_2, \cdots, n_k$) and l system measures (e.g. $m_1, m_2, \cdots, m_l$), a weighting coefficient α_i, $i \in [1, l]$ is assigned to each of system performance measures. Given a variable vector a, the weighted product P is calculated as follows

$$P(a) = \left[m_1(r)\right]^{\alpha_1} \left[m_2(r)\right]^{\alpha_2} \cdots \left[m_l(r)\right]^{\alpha_l} = \prod_{j=1}^{l} \left[m_j(r)\right]^{\alpha_j} \qquad (2)$$

For any two variable vectors a_1 and a_2, if $P(a_1) > P(a_2)$ can be obtained, it can be concluded that $a_1 > a_2$ i.e. the variable vector a_1 is better than a_2.

3. Pervious Concrete

3.1. System descriptions

A mix design of concrete is usually given as the relative ratios of the weights of all ingredients, i.e. $w = 1 : r_{wc} : r_{a_1c} : r_{a_2c} : \cdots : r_{a_nc}$ where r_{wc} is water-to-cement ratio and r_{a_ic}, ($i \in [1, n]$), is the weight ratio between the i-th aggregate and cement. The ratio $1 : r_{wc} : r_{a_1c} : r_{a_2c} : \cdots : r_{a_nc}$ implies one part (by weight) of cement, to r_{wc} parts of water, to r_{a_1c} parts of aggregate a_1, until r_{a_nc} parts of aggregate a_n. For simplicity, in the proposed porous concrete system, the mix design w is expressed as a ratio vector $r = (r_0, r_1, r_2, \cdots, r_n)$ where $r_0 = r_{wc}$ and $r_i = r_{a_ic}$. Note that, because the ratio of cement to itself is constantly one, its value is not included in the ratio vector r. Then the ratio vector r is used as the system variable vector and the system utility function is denoted by $U(r)$ [3,4].

Now the problem seeking the optimal mix design w^* has been converted into the problem finding the optimal ratio vector r^* which maximizes the overall system utility, $U(r^*)$. Moreover, it is assumed that each ratio r_i, ($i \in [0, n]$), can only take finite discrete values within the given space R_i, i.e., $r_i \in R_i$ where $R_i = (r_{i1}, r_{i2}, \cdots r_{ik})$, $r_{i1}, r_{i2}, \cdots r_{ik} \in [r_i^{\min}, r_i^{\max}]$ and $r_i^{\min}$ and $r_i^{\max}$ are the minimum and maximum boundaries of space R_i. Thus the space of ratio vectors is $R = R_1 \times R_2 \times \cdots \times R_n$. Once the optimal ratio vector r^* is determined, the optimal value of utility function is derived and the weights of cement and other components can be easily derived.

3.2. Implementation of the Gibbs sampling method

Let $T = \{1, 2, \cdots\}$ denote the index of a sequence of iterations. At the first step $t = 1$, an arbitrary ratio vector denoted by $r(t)$, ($r(t) \in R$), is select. When the iteration moves from t to $t+1$, ($t \in T$, $t+1 \in T$), the ratio vector is updated from $r(t)$ to $r(t+1)$, i.e., the system state transits from $r(t)$ to $r(t+1)$. In this process, there is one and only one element r_i in $r(t)$, is updated according to the probability distribution $\Lambda_i(r_{-i}(t))$ as given below.

$$\Lambda_i(r_{-i}(t)) = \Lambda_i(r_i \mid r_{-i}(t)) = \frac{\exp\left(\frac{-b}{U(r_i, r_{-i}(t))}\right)}{\sum_{r_i' \in R_i} \exp\left(\frac{-b}{U(r_i', r_{-i}(t))}\right)}, \forall r_i \in R_i \qquad (3)$$

where β is a positive constant and

$$r_{-i}(t) = \begin{cases} r_0(t) & \text{if } i = 1, \\ r_1(t) & \text{if } i = 0. \end{cases} \qquad (4)$$

according to the observation of $r_{-i}(t)$. After updating the ratio from $r_i(t)$ to $r_i(t+1)$, the value of utility function $U(r(t+1))$ is evaluated for the new generated ratio vector $r(t+1)$. From (4), the value of r_i inducing a high $U(r_i, r_{-i}(t))$ deserves a high probability to be employed. Then the process moves forward to next iteration. Please note that, at any step t of the iteration process, system keeps tracking the average value of utility function $\overline{U}(t)$ and compare it with $U(r(t))$. If the difference between these values is equal or smaller than a pre-defined value ε and remains stable, the system converges. The average value of utility function $\overline{U}(t)$ is calculated as follows.

$$\overline{U}(t) = \frac{1}{t}\sum_{t'=1}^{t} U(r(t')) \qquad (5)$$

In the design of utility function $U(r)$ of pervious concrete, the pervious concrete system can be treated as a multi-criteria decision making (MCDM) problem which consists of l system performance measures. These l desired performance measures must be taken into account so that the system can reach the tradeoff among them. As mentioned in previous sections, the porosity in pervious concrete is produced by the reduction or the elimination of fine aggregate from the mix design of general concrete. As a result, the pervious concrete is featured with a high permeability rate. On the other hand, a high compressive strength is one desirable property of pervious concrete. Therefore, by using the weighted product model (WPM), the utility function U of the proposed system is defined as a function of compressive strength ($f_c(r)$ in MPa) and permeability rate ($K(r)$ in $mm/\sec$), i.e.,

$$U\left(f_c(r), K(r)\right) = \left[f_c(r)\right]^{\alpha_1}\left[K(r)\right]^{\alpha_2} \qquad (6)$$

where $\alpha_1 \in (0,1)$ and $\alpha_2 = 1 - \alpha_1$.

3.3. Convergence Analysis of the proposed system

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The proposed mix design optimization approach of pervious concrete can be modelled as a Markov chain. Given R as the space of the ratio vectors of the system and let r_{init} and r_{end} denote the initial and the end ratio vectors, respectively, the transition matrix is $P = \sum_{i=1}^{n} P_i$ where $P_i = p_i(r_{init}, r_{end})$, $\forall r_{init}, r_{end} \in R$, with

$$p_i(r_{init}, r_{end}) = \begin{cases} \Lambda_i(r_{end,i} \mid r_{init,-i}) & \text{if } r_{init,-i} = r_{end,-i}, \\ 0 & \textit{otherwise.} \end{cases} \tag{7}$$

where $r_{init,-i} = (r_{init,1}, \cdots, r_{init,i-1}, r_{init,i+1}, \cdots, r_{init,n})$ is defined as the same manner. In (8), $p_i(r_{init}, r_{end})$ indicates the transition probability between r_{init} and r_{end} of an iteration step with respect to the *i*-th element in the ratio vector. Based on this definition, it could be induced that there must exist such an integer k , $k > 0$, that, after k iterations, all ingredients (i.e. all elements in the ratio vector) have updated their ratios at least once. In other words, all the entries in $P^{k'}$, $k' > k$, are strictly positive, which corresponds to a regular Markov chain. Because a regular Markov chain is actually also an ergodic Markov chain, the Markov chain of the proposed system is an irreducible, aperiodic and positive recurrent Markov chain and has the convergence properties of an ergodic Markov chain. Moreover, the Markov chain of the proposed system must converge to the unique stationary distribution $\pi = (\pi_1, \pi_2, \cdots, \pi_{|R|})$ in which $|R|$ is the cardinality of R and π_r , $\pi_r \in \pi$ is defined as follows.

$$\pi_r = \frac{\exp(\frac{-b}{U(r)})}{\sum_{r' \in R} \exp(\frac{-b}{U(r')})} \tag{8}$$

Let r^* denote optimal ratio vector maximizing the utility function U . For simplicity of notation, we denote $U(r^*)$ by U^* which indicates the value of the utility function when the variable is the optimal ratio vector r^* . Note that, because r^* is the optimal ratio vector, the corresponding U^* is the maximum value compared with the values of $U(r)$ when $r \neq r^*$. Moreover, if there are more than one optimal ratio vector, we define R^* as the set of all optimal ratio vectors, i.e. $r_i^* \in R^*$, $i \in [1, |R^*|]$ .As a result, $U^* = (U_1^*, U_2^*, \cdots)$ is the collection of maximum values of utility function corresponding to $r_1^*, r_2^*, \cdots$, ($r_1^*, r_2^*, \cdots \in R^*$).

Dividing the numerator and the denominator of (9) by $\exp(\frac{-b}{U(r^*)})$ gives

$$\pi_r = \frac{\exp[-b\delta(r)]}{\exp[-b\delta(r_1)] + \exp[-b\delta(r_2)] + \cdots + \exp[-b\delta(r_M)]} \tag{9}$$

where $\delta(r) = (\frac{1}{U(r)} - \frac{1}{U^*})$.

Note that, when $r = r^*$, we could induce that $\delta(r^*) = (\frac{1}{U(r^*)} - \frac{1}{U^*}) = (\frac{1}{U^*} - \frac{1}{U^*}) = 0$. As a result, $\exp[-b\delta(r^*)] = \exp(0) = 1$. Thus,

$$\pi_r = \begin{cases} \dfrac{\exp[-b\delta(r)]}{1+\sum_{r'\in R, r'\notin R^*}[-\beta\delta(r')]} & \text{if } r^* \text{ is unique,} \\ \dfrac{\exp[-b\delta(r)]}{|R^*|+\sum_{r'\in R, r'\notin R^*}\exp[-b\delta(r')]} & \text{otherwise.} \end{cases} \qquad (10)$$

where $|\cdot|$ indicates the cardinality of $(\cdot)$. In (11), it can be observed that the value of b has great impact on the stationary distribution. Considering the general cases where $|R^*|>1$, we have

$$\lim_{b\to\infty}\pi(r) = \lim_{b\to\infty}\frac{\exp[-b\delta(r)]}{|R^*|+\sum_{r'\in R, r'\notin R^*}\exp[-b\delta(r')]} \qquad (11)$$

Note that $\lim_{\beta\to\infty}\exp[-b\delta(r')]=0$, $r'\in R$ and $r'\notin R^*$. If $r'\notin R^*$, then $\delta(r)=0$, and

$$\lim_{b\to\infty}\pi(r) = \lim_{b\to\infty}\frac{\exp[0]}{|R^*|+\sum_{r'\in R, r'\notin R^*}\exp[-b\delta(r')]} = \frac{1}{|R^*|} \qquad (12)$$

otherwise,

$$\lim_{b\to\infty}\pi(r) = \lim_{b\to\infty}\frac{0}{|R^*|+\sum_{r'\in R, r'\notin R^*}\exp[-b\delta(r')]} = 0 \qquad (13)$$

From (13) and (14), it can be found that the value of each element in the stationary distribution is primarily dominated by the coefficient b. It can be observed that the Markov chain of the proposed system must converge to a stationary distribution when the coefficient b approach infinite, as shown in (13) and (14).

4. Simulation Configurations and Results

4.1. Configurations

As a primary interest of pervious concrete research, the permeability is measured as the water penetrating through pervious concrete samples which is expressed in millimeters per second ($mm/\sec$). In our proposed system, we will use the experimental data provided in [] to build up the MCMC system model. According to the experimental data, the maximum compressive strength and the maximum permeability rate are $f_{c,\max} = 19.8573 MPa$ and $K_{\max} = 26.6630 mm/\sec$, respectively. In all simulations, it is assumed that, except cement, only water and one type of coarse aggregate sizes between $4.75mm$ and $9.5mm$ are used to make the pervious concrete samples. The water to cement ratio and the aggregate to cement ratio are denoted as r_0 and r_1, respectively. More specifically, the minimum and maximum values of these parameters are summarized in Table 1. Please refer to [3] for the detailed experimental data and more information on the configurations and preparations of the specimen.

By following (7), the maximum value of utility function can be obtained as follows

$$U_{\max} = U_{\max}(f_c(r), K(r)) = \max_{r\in R}\{[f_c(r)]^{\alpha_1}[K(r)]^{\alpha_2}\} \qquad (14)$$

Based on the configurations given above, a number of simulations are carried out to verify the effectiveness and efficiency of the proposed Gibbs Sampling approach.

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Table 1 Initial relative ratios of components

Components	Ratio	Min value	Max value	Steps
Cement	1	NA	NA	NA
Water	r_0	$r_0^{min} = 0.3$	$r_0^{max} = 0.4$	1000
Aggregate	r_1	$r_1^{min} = 3.1$	$r_1^{max} = 5.7$	1000

4.2. Simulation results

We first observe the effect of the controlling parameter b on the performance of the Gibbs Sampling method. Figure 3compares the compressive strength of the Markov Chain Monte Carlo based approach with the other two approaches, each of which focuses on maximizing either compressive strength or permeability rate only. It is shown that the Gibbs Sampling optimal mix design achieves the trade-off between a high compressive strength while maintaining a desired permeability rate. The figure suggests that a large value of b is preferable when it comes to the optimality of the solution.

Next, we evaluate the effect of the weighting coefficient α_1 on the performance of the system. The value of α_1 varies from 0 to 1 with 0.1 increment. Figure 4 shows the comparison of the compressive strength at different values of α_1. It can be observed that, when $\alpha_1 \in [0, 0.45]$, the compressive strength remains stable regardless the value of b. Thereafter, the value of compressive strength dramatically and almost linearly increases with the increase of α_1. Figure 5 shows that the permeability rate remains stable when $\alpha_1 \leq 0.45$. When $\alpha_1 > 0.45$, the permeability rate significantly decreases with the increase of α_1.

5. Conclusions

This paper proposed a Markov Chain Monte Carlo algorithm-based optimization algorithm to approximate the optimal mix design of pervious concrete. The derived optimal mix design achieves the trade-off between the maximum compressive strength and the desirable permeability rate of pervious concrete. We also proved that the proposed method effectively and efficiently converges to the optimal solutions. A control parameter b employed in the proposed algorithm dominates the speed and accuracy of convergence, specifically, a large value of b leads to a fast convergence speed and a high convergence accuracy. Simulations show the consistent results.

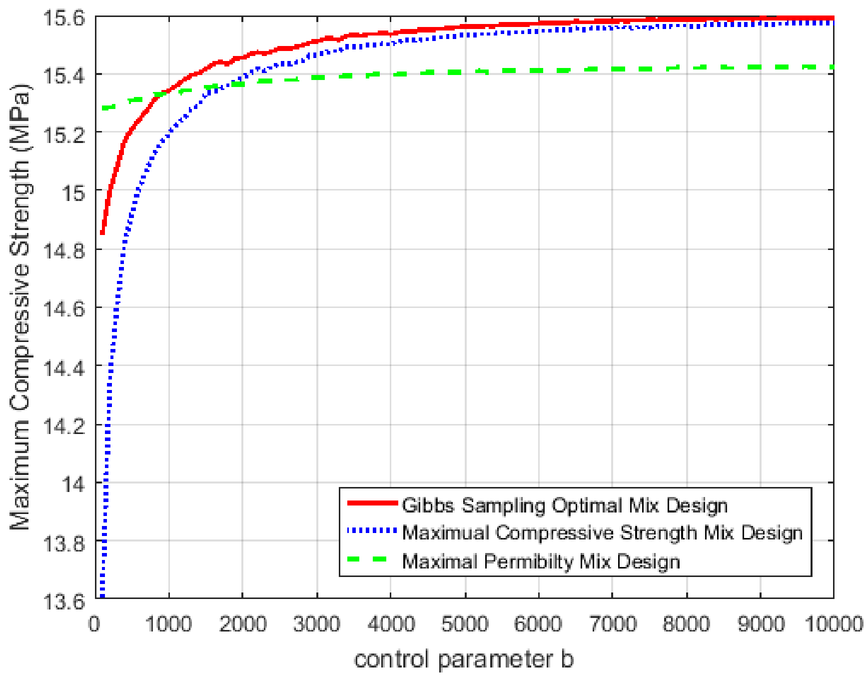

Figure 3. Compressive strength for different ***b***.

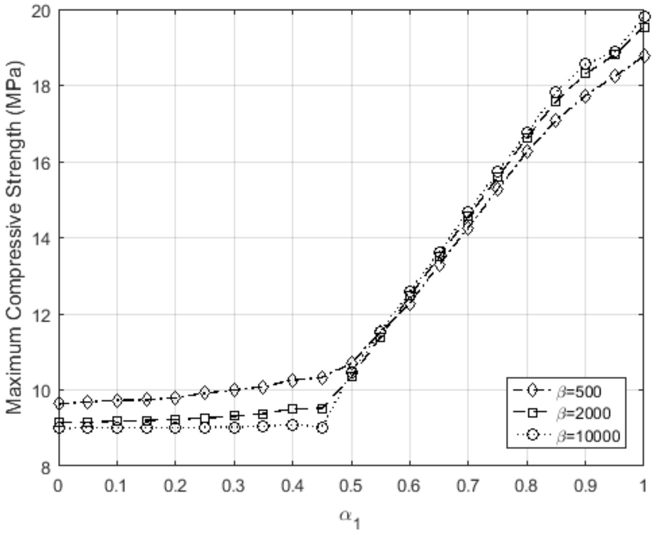

Figure 4. Compressive Strength for different $\boldsymbol{\alpha_1}$.

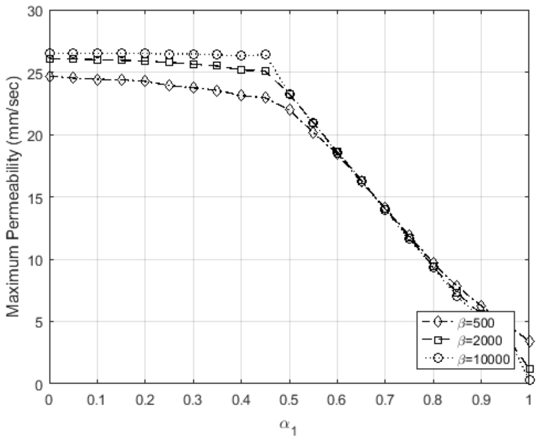

Figure 5. Permeability for different $\boldsymbol{\alpha_1}$.

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