Application of Monte-Carlo Simulations in Environment and Chemistry

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Abstract. Contemporarily, with the rapid development of the computer science, the calculation ability has been boosted a lot, which paves a path for carrying out simulations with random variable. In this case, Monte-Carlo simulations can be easily achieved with the state-of-art techniques. As one of the useful statistical tools, Monte-Calo simulation can be implemented in different areas including environment and Chemistry field. On this basis, this article searched several information to determine the usage of the simulation in the certain field. To be specific, the usage of Monte-Calo simulations of Chemistry and Environmental Science will be discussed with specific samples and data analysis. Moreover, relevant simulations results and corresponding applications will be demonstrated. In addition, this study will also summarize some limitations (e.g., the large range of the data). On this basis, it provides some suggests to elaborate the function in more digits and stating the conclusion. These results shed light on guiding further simulations in the context of the Monte-Carolo configuration.

Keywords: Monte-Calo simulation; Chemistry; Environment issues.

1. Introduction

Monte Carlo model is a stochastic simulation method. A calculation method based on the theoretical methods of probability and statistics. The approximate solution of the problem can be obtained by combining the problem with a certain probability model and using computer to realize statistical simulation or sampling. To symbolically show the probabilistic and statistical characteristics of this method.

In fact, the necessity of Monte-Carlo simulations will be demonstrated following. In order to know is there any affection of the rock grouting. The Monte-Calo simulation can be used for the numerical analysis model of random fractured rock mass grouting is established. As the result, the expanding distance increases as the time increases. The Monte-Calo simulation can analysis the distribution characteristics of fracture in the reconstructed surrounding rock and it also reflects the influence of fracture field on grouting reinforcement.

Lots of Environment Science and Chemistry areas need to prove some experiment through the huge amount of data like the mass of some elements or the area of a province. In this case, people cannot calculate all of them by once. Therefore, people will use Monte- Calo simulation to select some of the data and insert them in the equation to get the maximum, minimum and mean value of the data. On this basis, scholars can know the way that the rough results can be shown and represented of the whole case. After that, one can use the date to prove next step.

Regrading to the field of chemistry and plasma physics, lots of scholars investigate the role of plasma electrons, this paper uses Monte Carlo simulations. The results of the new model are closer to the experimental results, and the role of anodic plasma electrons cannot be ignored when describing the physical process of rod pinch diode [1].

Consider the effect of pulse stacking. Article obtained the photon counting distance measurement method based on PMT walking error, ranging precision and echo of laser pulse width, PMT output electron flow pulse width and photon event to identify the relationship between the threshold [2].

In order to further optimize the noise effect of the coupler, Monte Carlo simulation is used in this paper. The stability and refinement of the coupler are verified by the error rate of the results [3].

Since porous materials have strong absorbability, this paper intends to obtain the adsorption amount of mAlFu through Monte Carlo simulation so as to confirm whether it is possible to adsorb carbon dioxide through this material. The results show that the adsorption capacity of mAlFu is stable and has great application potential [4].

To investigate the effect of flocculation on the optics of nanofluids, Monte Carlo simulations are used to model multiple scattering between particles. The results show that the model can predict the optical properties of flocculating nanofluids [5].

Because LED light can cover a large area of human skin and treat the spot, but in order to understand the penetration of light waves, this paper uses Monte Carlo simulation to confirm the light distribution and energy absorption. It turns out that in different parts of the body, the diverging half Angle of the plate needs to be controlled within 30 degrees [6].

In order to know whether all of the aspects of Chemistry and Environment Science can use Monte-Calo simulation, this article will look through some of the specific cases about these two areas and to check is there any limitation or flaws. Therefore, the rest part of the paper is organized as follows. the next part will talk about the principle of Monte Carlo simulation. After that, it will be the analyze of the usage of Chemistry and Environment Science. Subsequently, the limitations of the current study and applications will be clarified and future outlooks will be proposed following the statements accordingly. In the last section, the conclusions and implications of the study will be discussed eventually.

2. Principle of Monte-Carlo simulations

Monte-Carlo simulations are the model that used for detecting the huge amount of data. It works for picking some data from a huge database and to calculate the minimum, maximum , the average and the meant. This simulation can work really fast and easily. It is a numerical simulation method which takes probabilistic phenomena as the research object. As a matter of fcat, it is a method of calculating unknown characteristic quantity by obtaining statistic value by sampling survey. The formulae of the average value and expected value of a certain function $f(X_i)$ with probability of $p(X_i)$ are given as follows:

$$\bar{x} = \sum_{i=1}^{n} \frac{x_i}{n} \tag{1}$$

$$F_N = \frac{1}{N} \sum_{i=1}^{n} \frac{f(X_i)}{p(X_i)} \tag{2}$$

3. Applications in environment

Since lots of coals and fossil fuels are burned, there are bunch of ashes be produced by the burning. The carbon dioxide and the green house gasses are produced through this process, which harm the environment. In addition, during the transmission period, the wind and the machine also led to the impact for the human health and environment pollution. Hence, in order to know and analyze the uncertainty of the ash, the Monte Carlo simulations are applied to test the realistic situation for the environment pollution.

To begin with, one constructed the new model:

$$F(x) = f(x)[1 + a] \tag{3}$$

The case in this article is about the central heating project. The area of coal yard is calculated according to 10D. The field area is $40m^2$, and the coal load is about 90T. The deterministic dust intensity calculation result is 20.3 mg/s. Dust strong degree is less than 20.3 mg/s in the probability is only 33.23%, dust strong degree is larger than 20.3 mg/s probability is 66.77%, and the intensity

of dust. In the probability of 50 mg/s is 18.10%. According to the intensity of dust range is (5.48, 87.06).

In daily environmental management, if a windbreak wall is installed to reducing the wind speed of coal field can effectively reduce the amount of coal dust. Uncertainty analysis based on Monte Carlo method can be generalized to other environmental models, which will provide valuable decision support for environmental protection departments [7].

As the huge output of Carbon in China, other scholars use the DICE model to test the trend of industrial carbon output and the global climate change. It also calculates Carbon emissions and the response of global temperature to shocks to general production and energy-related technologies. Run 1000 simulations to obtain trends in China's output, China's industrial carbon emissions and global atmospheric temperature changes [8].

As the result, all the variables increase and have the same trends. This means the higher productivity cause the more Carbon emission and the higher global temperature. Simulations suggest that 50 years from now global temperatures will be about 2 degrees Celsius warmer than in 2000. Global temperatures and China's carbon emissions are rising exponentially [8],

Other researchers also carried out analysis on the value measurement model of carbon emission rights, which is to prove the possibility that the economic field can drive environmental protection. In this case, the Monte Carlo model was used to run 1000 tests to get the probability distribution and sensitivity analysis of the model and also to die to value and environmental capacity of carbon emission rights refer to the price [9].

The results show that for the CO_2 absorption cost of carbon sink, the A-D value of Beta distribution 0.4758 is the lowest and the goodness of fit is the highest. The median value of the fitting result is 451.86 yuan/ton, and the expected value is 489.44 yuan/ton as shown in Fig.1.

The theoretical carbon pricing model proposed in this paper fully takes into account the specific national conditions of each country and conforms to the framework of common but differentiated responsibilities in addressing climate change.

4. Applications in Chemistry

In order to know can EAM model identify the silver's saturated vapor pressure, the article use the EAM, MC simulation and the NVT system. Researchers   calculate the saturated vapor pressure of silver from 1700k-2300k. The calculated results show that the error between the simulated results and the measured saturated vapor pressure is within 30% at all temperatures. That means the EAM model of silver can extend to the gas phase simulation.

The MC program was used to calculate the average energy, pressure and chemical potential of particles at temperatures ranging from 1700K to 2300K, and the acceptance ratio calculated by MC was output as summarized in Table. 1. Seen from the results, the error between the results and the experimental measurement is within 30%. The saturated vapor pressure of Ag is described reasonably and successfully by the embedded atom theory. The potential energy model can be extended from the simulation of liquid state to the simulation of gas state [10].
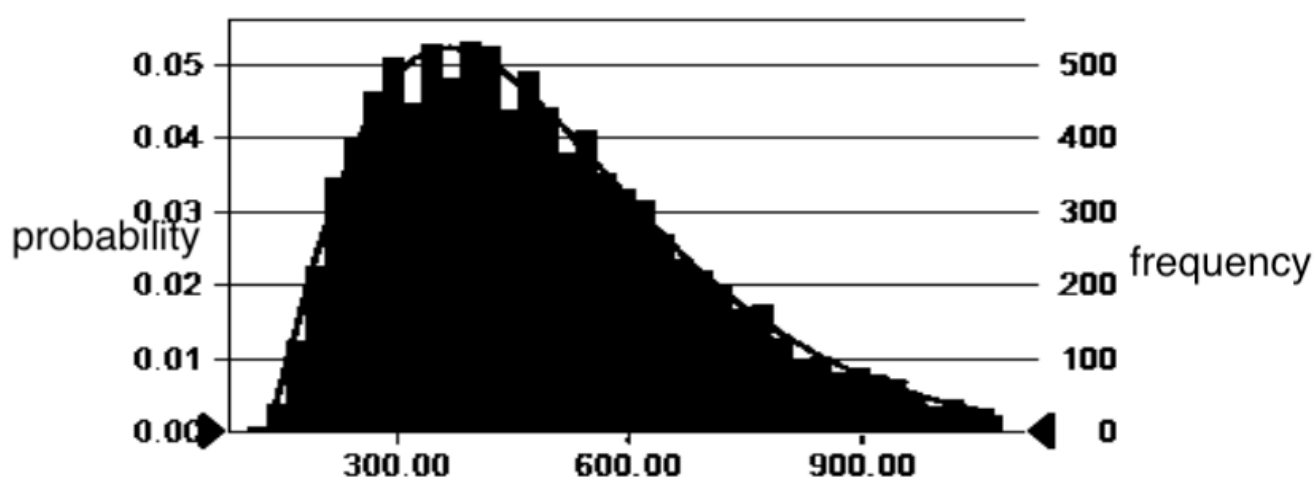
Fig. 1 Frequency distribution and probability density map of CO2 absorption cost of carbon sink

**Table 1**. The result of 2300k that under the MC simulation

Density (g.cm^{-3})	Atom Density (#.A^{-3})	Average Energy (k$_b$T/#)	Pressure (bar)	Chemical Potential (nk$_b$T)	Acceptable rate Percent
7.09	0.03956	-11.36945	-562.99524	-23.78499	64.362
7.11	0.03967	-11.37904	-269.44307	-23.79679	64.336
7.13	0.03978	-11.40205	133.39516	-23.77607	64.133
7.15	0.03989	-11.39404	144.03006	-23.75141	64.235
7.17	0.04000	-11.41392	327.15307	-23.75447	64.18
7.19	0.04011	-11.41929	599.53838	-23.72222	64.015
7.21	0.04023	-11.43256	611.22885	-23.69618	64.025
7.23	0.04034	-11.44355	977.22046	-23.66385	63.921

Monte Carlo simulation method is also applied to the prediction of lead-zinc-Ag deposits in stratified carbonate rocks in Liaoning Province. The quantity of basic samples or units participating in Monte Carlo simulation and the size of the favorable coefficient have an important impact on the simulation results. Therefore, the selection of units for Monte Carlo simulation should have ore units to ensure the reliability of the prediction results [11].

Since the adsorption capacity of shale is determined by things (e.g., pore structure). Therefore, one did a molecular simulation of methane adsorption using the Monte Carlo method, and it is wanted to see the effect of pressure and temperature on adsorption. The results show that the adsorption capacity decreases with the increase of temperature and increases with the increase of pressure [12, 13]. The typical structures of pores and snapshots of the structure are illustrated in Fig. 2 and Fig. 3.

Fig. 2 Typical sketch of different kinds of pores.
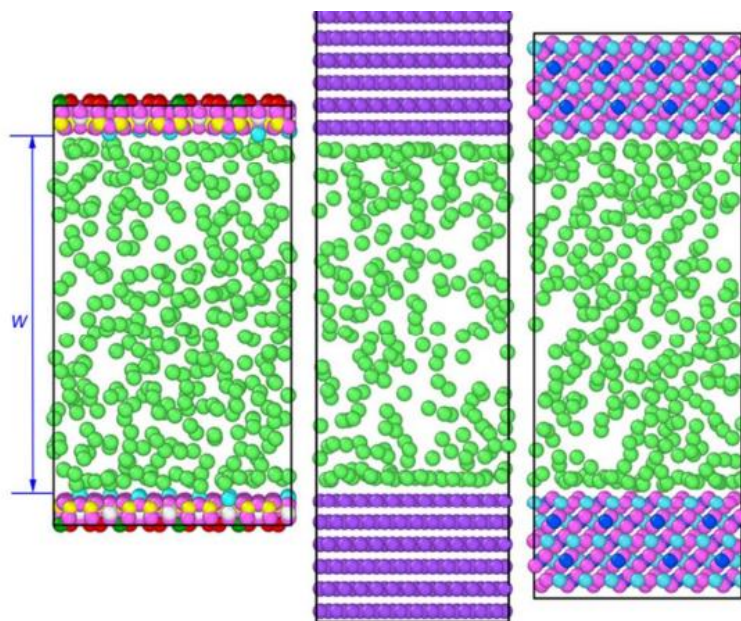
Fig. 3 A snapshot of the sturctures.

This paper mainly uses graphene and $C_5H_4O_2$ for molecular simulation as summarized in Table. 2. The relationship between these two substances and the pressure can be showed

$$n_{ab} = n_0 \left(\frac{p}{p_0}\right) \alpha \times \left(1 - \frac{T}{|T_0|}\right) \beta \tag{4}$$

The results show that when the pressure is low (≤2MPa), methane molecules are mainly distributed in the area near the pore wall, and methane molecules mainly exist in the form of adsorption state. When the pressure is high (2MPa), the methane molecules in the pore wall and the central region increased rapidly, and methane molecules exhibited adsorption and free states at the same time. The density of methane molecules in both adsorbed and free states increases with the increase of pressure, but the proportion of methane molecules in adsorbed states decreases gradually with the increase of pressure [14].

Table 2. Absorption constants of organic matter nanopore

Pore	$n_0/(mmol/m^2)$	α	β
Graphene	0.00273	0.559	0.985
$C_5H_4O_2$	0.00244	0.566	0.970

5. Limitations & Prospects

In some cases, the huge amount of the variables and the huge amount of assumption data may lead the inaccuracy of the result. Sometimes, it may hard to determine how many data need to be used to insert in the Monte-Carlo simulation. For some of the cases, people set the conclusion all base on the assumption, which they pick the data randomly and lead the deviation for some result. In addition, Monte-Carlo simulation sometimes needs to rely on other models to test its accuracy.

In the future, people are willing to see more application is more areas. Scholars can get the more accurate value that with less data and less deviation. Moreover, it is important for people to gain a database that has high accuracy. As people are using the Monte-Carlo simulation, they can insert some of the data that mainly affect the result and get the most specific answers under the using of the simulation. They also do not need to rely on other equations or other simulations to proof their result again. In addition, people are willing to see that whether Monte-Carlo simulation can select the data automatically and the inner function and work more specific, which can provide more digit for people to obtain the result that close to the truth.

6. Conclusion

In summary, this paper mainly investigate the Monte-Carlo simulation based on the Cheemistry and Environmental Science aspects. To be specific, Monte-Carlo simulation has a widely using in some areas. It based on some random data and then insert then to the equation to get the range of the final result. In this paper, it is mainly talked about the usage of Monte-Calo simulation in Chemistry and Environmental Science regions. According to the analysis, lots of the chemistry experiment using the Monte-Carlo simultion to prove the exact range of their arguement . Besides, in Environment Science region, the Monte-Carlo simulation can be used to determine the pollution level of an area and which can help to decide whether the area need to be protect or not . Nevertheless, Monte-Carlo simulation has some limitations like they need to rely on other simulations to proof it accuracy and it cannot be widely used under some special situation. In the future, Monte-Carlo simulation may be more accurate , which can select the most effective data from the database to get the more accurate and more specific result for researchers. Overall, these results offer a guideline for the application of the Monte-Carlo simulation.

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