

## Article

# Improving Ammonia Emission Model of Urea Fertilizer Fluidized Bed Granulation System Using Particle Swarm Optimization for Sustainable Fertilizer Manufacturing Practice

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**Abstract:** Granulation is an important class of production processes in food, chemical and pharmaceutical manufacturing industries. In urea fertilizer manufacturing, fluidized beds are often used for the granulation system. However, the granulation processes release ammonia to the environment. Ammonia gas can contribute to eutrophication, which is an oversupply of nitrogen and acidification to the ecosystems. Eutrophication may cause major disruptions of aquatic ecosystems. It is estimated that global ammonia emissions from urea fertilizer processes are approximately at 10 to 12 Tg N/year, which represents 23% of overall ammonia released globally. Therefore, accurate modeling of the ammonia emission by the urea fertilizer fluidized bed granulation system is important. It allows for the system to be operated efficiently and within sustainable condition. This research attempts to optimize the model of the system using the particle swarm optimization (PSO) algorithm. The model takes pressure (Mpa), binder feed rate (rpm) and inlet temperature (°C) as the manipulated variables. The PSO searches for the model's optimal coefficients. The accuracy of the model is measured using mean square error (MSE) between the model's simulated value and the actual data of ammonia released which is collected from an experiment. The proposed method reduces the MSE to 0.09727, indicating that the model can accurately simulate the actual system.

**Keywords:** particle swarm optimization; ammonia emission; granulation; urea fertilizer



**Citation:** Mohamad, N.; Ab. Aziz, N.A.; Ghazali, A.K.; Salleh, M.R. Improving Ammonia Emission Model of Urea Fertilizer Fluidized Bed Granulation System Using Particle Swarm Optimization for Sustainable Fertilizer Manufacturing Practice. *Processes* **2024**, *12*, 1025. <https://doi.org/10.3390/pr12051025>

Academic Editors: Chia-Nan Wang, Nhat Luong Nhieu, Phan Van-Thanh and Hector Tibo

Received: 28 March 2024

Revised: 1 May 2024

Accepted: 2 May 2024

Published: 18 May 2024



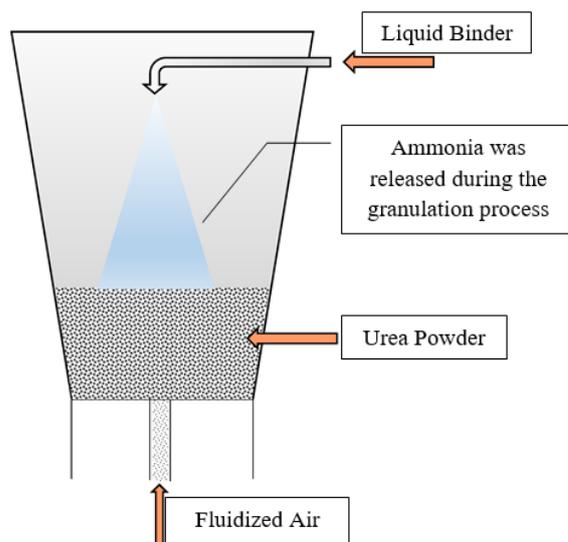
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## 1. Introduction

Granulation is an important step in the manufacturing process of food, chemicals and pharmaceuticals. It is used to make the individual solute particles in fluid mixtures flock together in bigger entities called grains or granules. Granulation occurs through the creation of bonding between the solid powder particles. The bonding of the powder particles can be induced through the application of a binding agent. The transformation of the powder particles into granules allows the tableting process to produce tablets of required quality at the required tablet press speed range [1,2]. The granulation process is also instrumental in urea fertilizer production. Urea fertilizer stands out as the most widely utilized solid nitrogenous fertilizer globally due to its excellent water solubility [3,4]. Compared to other nitrogenous fertilizers, urea provides a higher quantity of nitrogen to plants and soil owing to its concentrated nitrogen content of 46%. In Malaysia, urea fertilizer subsidies are provided by the government to assist farmers in gaining better productivity [5]. The effectiveness of urea-based fertilizer in improving productivity and yield of maize and paddy is reported in [6] and [7], respectively.

Although urea is proven to be a good fertilizer, its usage and production pose risks to the environment, including the release of ammonia gas. A study conducted at paddy field of Jiangxi Province China from 2019 to 2021 observed that ammonia volatilization

increases after fertilization [8]. Another study from China, which was conducted at the Jiangsu Province from 2000 to 2017 in [9], reported that among the main cause of ammonia emissions by agriculture sector is the nitrogen fertilizer. Specifically, urea and ammonium bicarbonate from nitrogen fertilizer contribute around 80% of the ammonia emissions. In addition to the emission from the application of the fertilizer itself, the urea granulation process also contributes to ammonia emissions. Figure 1 shows the reaction process of fluid bed granulation where the ammonia gas is released during the mixing of urea powder with the urea binder solution. The ammonia gas is formed when the urea solution is heated under high pressure. The ammonia gas is released to the environment through the output ventilation from the fluid bed granulation's chamber.



**Figure 1.** Schematic of fluidized bed granulation process.

The ammonia gas can be highly poisonous and has a multitude of impacts on a variety of live beings [10]. For humans, inhaling ammonia vapor poses risks such as irritation and corrosive damage to the skin, eyes and respiratory tracts. Inhalation of very high levels can even be fatal. When dissolved in water, the elevated levels of ammonia are also toxic to a wide range of aquatic organisms. Ammonia can also contribute to eutrophication, an oversupply of nitrogen and acidification to the ecosystems.

Optimal manufacturing of urea fertilizer is important. It not only helps to improve effectiveness of the urea absorption for better plant growth [11], but also minimizes the negative impact to the environment including the amount of ammonia gas pollution. Therefore, this research focuses on minimizing the amount of ammonia gas released by the urea fertilizer fluidized bed granulation system without affecting the quality of urea granules. This is achieved through the utilization of optimal modeling of the fluidized bed granulation system. Mathematical modeling is popularly used across all fields to represent a system or a process. For example, the modeling of capacitance of a supercapacitor is discussed in [12], the spraying process of an electrostatic oiling machine is modeled in [13] and the model of reservoir operation is reported in [14].

Here, urea fertilizer fluidized bed granulation system model parameters are optimized using particle swarm optimization (PSO) with three manipulated variables, namely pressure (Mpa), binder feed rate (rpm) and inlet temperature ( $^{\circ}\text{C}$ ). The readers are referred to our earlier work [15] for details on the previously developed model using the Response Surface Method (RSM). The developed model is using a quadratic polynomial model. RSM is popularly used for modeling. It is useful in finding empirical relations and the effect of each parameter and their interactions on the responses considered [16]. In [17], an attempt was made to study radial gas mixing in a fluidized bed using RSM to determine

the relationship between radial gas mixing and operating conditions in the bubbling or slugging fluidization regimes.

In this work, the modeling problem is formulated as a 10-dimensional minimization problem with PSO [18] is used as the optimizer. PSO is frequently used in optimization of a mathematical model. PSO is used for parameter optimization of a simulated biological system in [19]. In another work [20], PSO is used to model the pH of a hydroponics system for better plant growth. PSO is also used for optimizing the susceptible, infected and resistant (SIR) models of infections in [21]. In [22,23], PSO is used for the optimization of parameters of a controller system model. Meanwhile, PSO is used for modeling of a single link flexible manipulator in [24]. These works show that PSO is a powerful algorithm towards optimizing and improving mathematical models. PSO is a black box modeling technique that is simpler compared to the traditional method [24]. Additionally, the traditional modeling method is more suitable for a linear system [22]. The success of PSO in optimum modeling of various systems and its advantages motivates this research. The optimized model of the fluidized bed granulation system is validated by comparing the simulation data with the experiment data. The model's best mean square error (MSE) is 0.09727, which shows the high accuracy of the model.

This work is presented in four sections. The methodology is presented in Section 2. The experimental setting is discussed in Section 3. This is followed by the results and discussion section. Lastly, the work is concluded, and future direction is discussed in Section 5.

## 2. Related Works

Mathematical modeling of fertilizer systems had been adopted by existing works for various perspectives. For example, Lipin et al. [25] created an inclusive model to forecast nutrient release from controlled release fertilizers (CRF) that incorporates all three release stages: (1) the initial stage of liquid infiltration in the coating layer, (2) the constant release stage where solid fertilizer exists in the core and (3) the gradual decay release stage when there is no more solid fertilizer in the core. This model consists of the computation of three coefficients: the water and nutrient diffusion coefficients within the coating layer as well as the coating material's limiting water absorption capacity. It provides the capacity to predict the rate of nutrient release, the cumulative release pattern for all release phases and coating types, presuming a diffusion-based release mechanism. The model reveals accurate simulation of nitrogen release from polymer-coated particles by investigating various coated urea types. It also predicts moisture content profiles and nutrient solution concentration profiles within the coated layer for lag, linear and decay times, as well as nutrient concentration in the aquatic environment.

Guo et al. [26] proposed mathematical models to describe the synthesis of urea–formaldehyde fertilizers with varying nitrogen release properties. This research employs a central composite design (CCD) of response surface methodology to investigate the impact of reaction times, temperatures and molar ratios on the solubility of nitrogen in hot or cold water. The results indicate that the solubility of nitrogen in water, whether cold or hot, from urea–formaldehyde fertilizers is mostly influenced by the molar ratios of urea to formaldehyde. Additionally, mathematical models based on quadratic polynomials are developed for urea–formaldehyde. The model is beneficial towards precise synthesis of urea–formaldehyde fertilizers. Similarly, nutrient release by spherical coated fertilizer granules was modeled in [27]. The model takes into consideration the granule's radius, contact area and diffusivity towards the fertilizer saturation and release time.

Meanwhile, an approach that focused on modeling the effectiveness of ridge–furrow film mulching and nitrogen fertilizer towards improving maize production quality was proposed in [28]. The model was developed using data collected in Loess Plateau, China. The authors reported that optimization of the model parameters contributes towards accurate modeling the maize grain filling process at different application rates of the fertilizer. The effectiveness of nitrogen, phosphorus and potassium fertilizer application

for growth of HB16 winter cauliflower is modeled in [29]. The model can determine the optimal fertilizer usage for achieving production target. This helps sustainable agriculture practice and avoids waste.

A review paper by Irfan et al. [30] highlighted the importance of mathematical modeling in developing more efficient fertilizers and understanding the release of nutrients from controlled release fertilizers (CRFs). The research emphasized how mathematical modeling may be used to anticipate and visualize nutrient release characteristics. It also stressed the need to have an extensive knowledge of the physiological and chemical processes that lead to nutrient release. Two categories of models are differentiated: mechanistic models and empirical models. The mechanistic models look into the coating material and nutrient contained inside the granule, while empirical models focus on moisture and temperature. On the other hand, Haydar et al. [31] in their review focused on the model for physiochemical parameters for slow and controlled release nanofertilizers such as the water retention and absorption capacity, the swelling ratio, the loading and nutrient use efficiency and several other parameters. The models offer quick predictions without the need to conduct actual experiment, thus providing time- and cost-effective solutions.

Swain et al. [32] investigated the performance of six machine learning algorithms, support vector machine, artificial neural network, random forest, M5 tree (M5P), reduced error pruning tree (REPTree) and surface response, in predicting and optimizing nitrate leaching from urea super granules (USGs). They explored various factors such as binding materials, binding agents and coating curing times as primary predictors. Some algorithms exhibited high efficacy in predicting nitrate leaching, but there is potential to enhance these models further by incorporating advanced optimization methods like genetic algorithms and particle swarm optimization. High prediction accuracy helps in determining the best amount of fertilizer to be used which is cost effective as well as reducing risk of pollution via nitrate leaching.

In contrast to the works reviewed above, the work by Duffuan [33] explored another angle of modeling for ammonia and urea fertilizer manufacturing. The author explored the modeling of federate with respect to the cost of the fertilizer manufacturing operation. The author reported that the model can help in choosing the best setting that helps in reducing the operational cost of the fertilizer plant.

Although there has been notable advancement in fertilizer modeling such as the release of nutrients, there is still limited work that focuses on modeling the manufacturing process of fertilizer, especially modeling the impacts of the manufacturing process on environment, specifically ammonia release. Moreover, in optimizing the models, an optimal model is expected to make a significant contribution to formulating the best sustainable manufacturing practice.

### 3. Materials and Methods

#### 3.1. The Mathematical Model of Fluidized Bed Granulation System

The mathematical model is developed based on the lab scale fluidized bed granulation shown in Figure 2a, whilst the schematic diagram of the system is shown in Figure 2b. In the schematic diagram, Section (1) is the granulator chamber, Section (2) is the ammonia measure channel and Section (3) is the binder feed line.

A quadratic polynomial model is used to model the system in the study using RSM [15]. The general form of the quadratic equation model is shown in Equation (1) below,

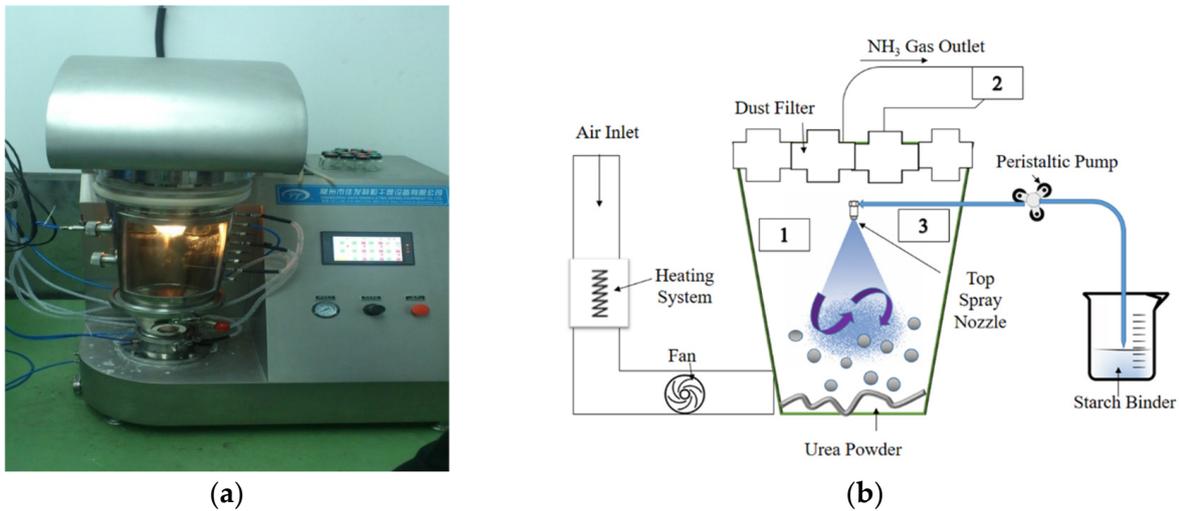
$$Y = \alpha_0 + \sum_{i=1}^n \alpha_i X_i + \sum_{i=1}^n \alpha_{ii} X_i^2 + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \alpha_{ij} X_i X_j, \quad (1)$$

where  $Y$  is the objective function or response which is the amount of ammonia release while  $X_i$  are operating parameters or factors. The number of parameters is represented by

*n*. In this work, there are three parameters: pressure (Mpa), binder feed rate (rpm) and inlet temperature (°C). Thus, the Equation (1) can be written as Equation (2):

$$Sim = a + bx + c(x^2) + dy + e(y^2) + f(z) + g(z^2) + hxy + ixz + jyz \quad (2)$$

Based on Equation (2), the symbols of *x*, *y* and *z* represent the temperature, binder volume and pressure, respectively. *Sim* is the predicted ammonia released by the model. The coefficient values *a*, *b*, *c*, *d*, *e*, *f*, *g*, *h*, *i* and *j* in Equation (2) are chosen here by PSO.



**Figure 2.** (a) Lab scale fluidized bed granulation system. (b) Schematic diagram of the system.

### 3.2. Model Optimization Using PSO

PSO is a swarm intelligence algorithm where a group of particles work together to search for the optimal solution. In this case, these are the coefficient values of the polynomial equation.

The algorithm of PSO starts with random initialization of the population. Here, the particles are randomly initialized between 0 and 1. After random initialization, the algorithm enters the iterative procedure of velocity and position update. The particle's velocity,  $v_{id}$ , is updated according to Equation (3).

$$v_{id} = \omega v_{id} + c_1 r_{1id} (p_{id} - x_{id}) + c_2 r_{2id} (p_{gd} - x_{id}) \quad (3)$$

$$\omega = -\frac{\omega_{max} - \omega_{min}}{\max\_iter} + \omega_{max} \quad (4)$$

Subscripts *i* and *d* in the equation represent particle number and parameter numbers, respectively. Since the model here has 10 coefficients to be optimized,  $d = \{1, 2, 3, \dots, 10\}$ .  $c_1$  and  $c_2$  are cognitive and social coefficients. They control the influence of the particle's own best experience  $p_{id}$  and the swarm's best solution so far,  $p_{gd}$ . Typically, both values are set to 2, giving balance influence. Inertia weight  $\omega$  controls the momentum of the particle from previous search. Linear decreasing inertia weight is adopted in this work to encourage exploration during the initial search process and later switch to fine tuning. The equation for inertia weight update is shown Equation (4), where  $\omega_{max}$  and  $\omega_{min}$  are the maximum (start) and minimum (end) values of inertia weight and  $\max\_iter$  is the number of iterations of the algorithm. PSO is a stochastic algorithm. The randomness of the algorithm is presented by random values  $r_{1id}$  and  $r_{2id}$  between 0 and 1.

Velocity is used to update the particle's position,  $x_{id}$ , which is shown in Equation (5).

$$x_{id} = x_{id} + v_{id} \quad (5)$$

The particle  $i$ th position represents a potential solution. The iterative procedure of updating the particle's velocity, position and fitness evaluation continues until the stopping condition is reached, which is the maximum iteration number. The PSO algorithm is shown in Figure 3.

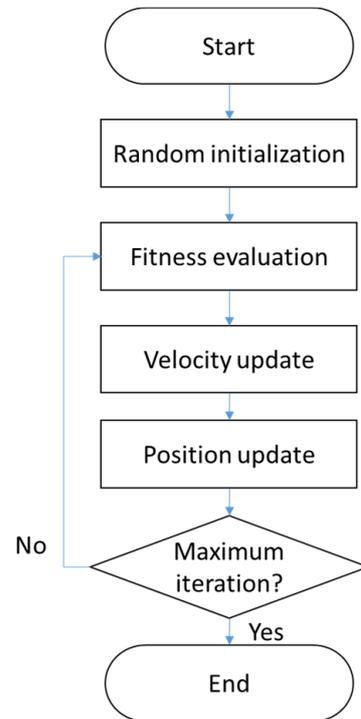


Figure 3. PSO algorithm.

### 3.3. Particle Encoding

The PSO particles are encoded according to the modeling problem to be optimized here. Each dimension of a particle represents a parameter in the model (Equation (2)). Particle encoding is illustrated in Figure 4.

$x_{i1}$	$x_{i2}$	$x_{i3}$	$x_{i4}$	$x_{i5}$	$x_{i6}$	$x_{i7}$	$x_{i8}$	$x_{i9}$	$x_{i10}$
$a$	$b$	$c$	$d$	$e$	$f$	$g$	$h$	$i$	$j$

Figure 4. Encoding of particle  $i$ .

### 3.4. Fitness Function

The fitness of quality of the solution proposed by PSO is evaluated using mean square error (MSE) shown in Equation (6).

$$MSE = \frac{1}{N} \sum_{k=1}^N (Y_{act,k} - Sim_k)^2 \quad (6)$$

In Equation (6),  $N$  represents the amount of data from the experiment conducted to measure the ammonia released,  $Y_{act}$ , by the lab scale fluidized bed granulation system. The objective of PSO is to minimize MSE to a value closer to 0.

## 4. Experimental Setting

Based on the design of the experiment (DOE), the potential ammonia released was collected for modeling the fluidized bed granulation system. The data were obtained through continuously injecting the binder liquid into the blended urea powder at a temperature between 40 °C and 95 °C. The injected blended urea powder was agglomerated and

transformed into urea granules. Approximately 75% of the binder liquid that was heated under the vacuum chamber at these pressure ranges produced a vapor and formed urea granules. The remaining urea powder and air supplied from the fluidized bed granulation were then removed from the machine into the ventilation outlet using the fan. The urea with the water solution then was discharged as ammonia to the atmosphere.

The urea powder in the chamber emitted as ammonia when it was exposed to the high pressure and temperature. The binder feed rate was set to two settings: 4 rpm and 6 rpm. The fluidized bed pressure was set to 200 kPa, 400 kPa and 600 kPa. The mixture was heated and temperature was consistently increasing throughout the urea granulation process, which released ammonia into the environment. The ammonia readings were continuously collected for every single minute interval. In total, 238 readings were recorded. The collected readings are reported in units of ppm. The readings showed that there was gradual increase in the amount of ammonia gas released from this process until it reached a temperature of 65 °C, and a downward trend was also shown afterward due to the depletion of urea binder reagents. The collected ammonia released value was used for the data points of modeling the system.

PSO was implemented using MATLAB. The parameters used for the modeling are shown in Table 1. The algorithm was run 30 times; average and best results were recorded.

**Table 1.** PSO parameter values.

Parameter	Value
No. of particles	30
Max. iteration, <i>max_iter</i>	5000
$\omega$	0.9–0.5 (linear decreasing)
$[c_1, c_2]$	[2, 2]

## 5. Results and Discussion

The MSE of the swarm's best at the end of iteration for each run is recorded. The average of MSE for the 30 runs is 24.2435. The best solution found by PSO among all the run has an MSE of 0.0973, which is close to zero. The error range between the ammonia predicted by the best model and the actual data collected during the experiment is [0.0026, 0.9468]. The small MSE indicates the accuracy of the model in simulating the actual fluidized bed granulation system while the small range shows the stability of the model over various settings of the fluidized bed granulation system. The best MSE and the average MSE observed are presented in Table 2. The coefficients' values that offer the best MSE are shown in Table 3.

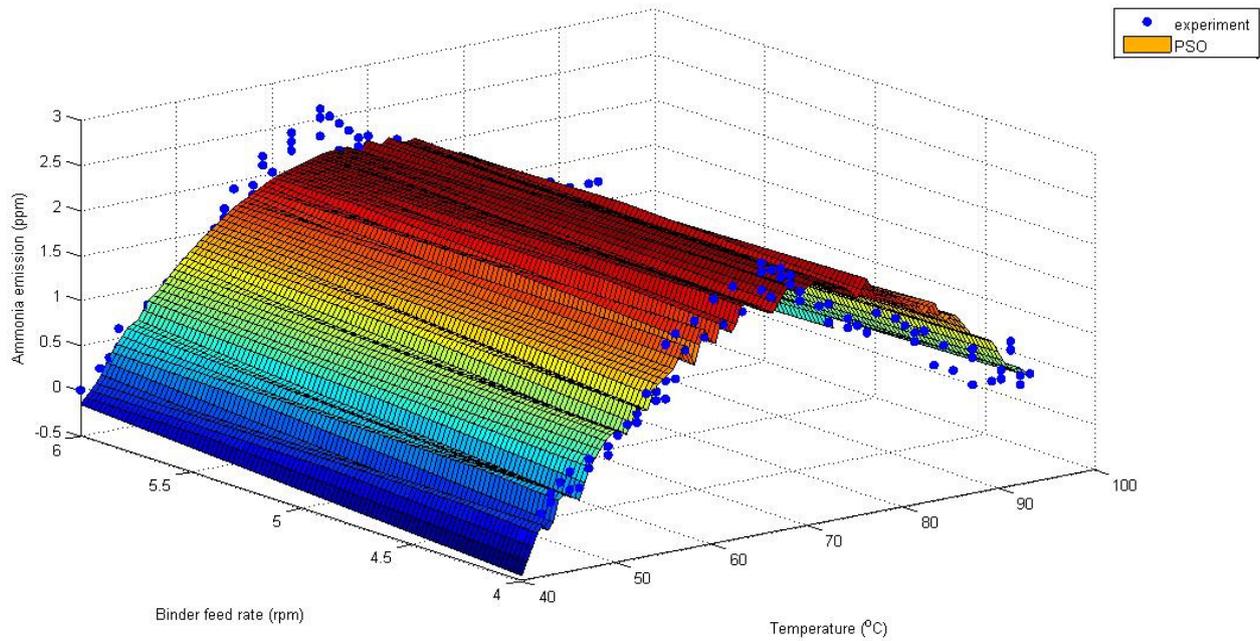
**Table 2.** MSE of the model.

Results	Value
Best MSE	0.0973
Average MSE	24.2435
Error range of the best model	[0.0026, 0.9468]

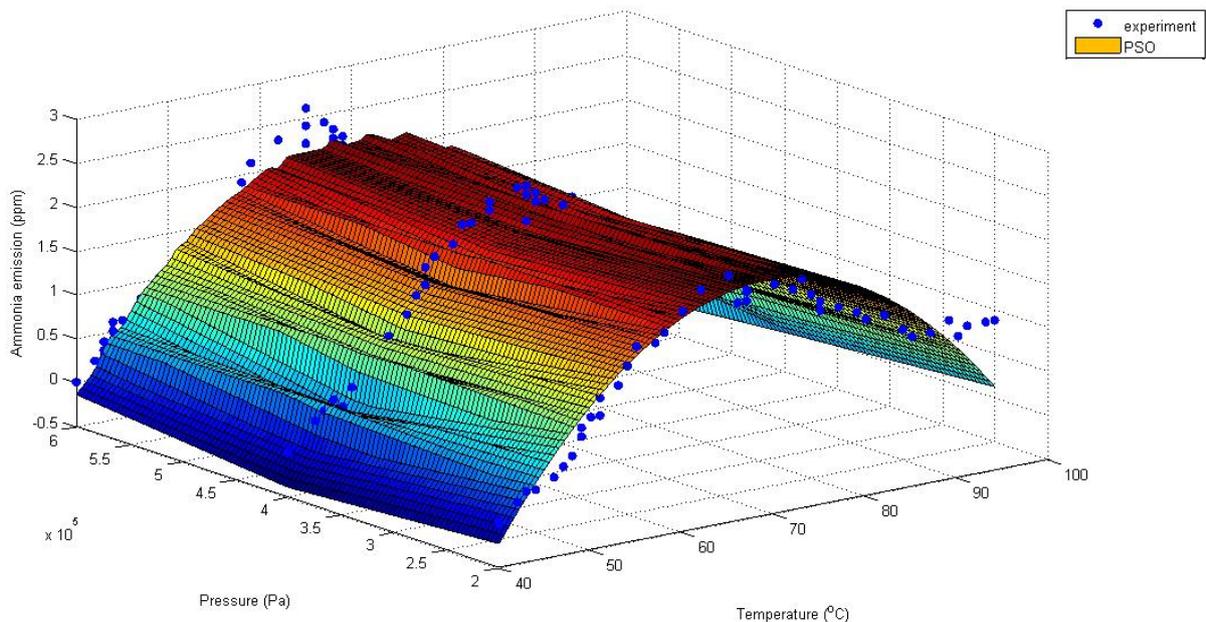
**Table 3.** Fit summary for model value.

<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>	<i>f</i>	<i>g</i>	<i>h</i>	<i>i</i>	<i>j</i>
0.0069	0.4576	1.0702	−2.9929	$1.0510 \times 10^{-10}$	$-6.6921 \times 10^{-5}$	−0.18571	$-9.3845 \times 10^{-7}$	$7.8564 \times 10^{-6}$	4.5556

Figures 5 and 6 show the surface plot of predicted ammonia release using the best model over temperature under different feed rate and pressure values. The data collected via the experiment are plotted in blue. The results show that the predicted values of ammonia gas released are significantly close with the actual data from the experiment. It is obvious from the graph that the predicted value from the model had a small discrepancy with the experimental data.



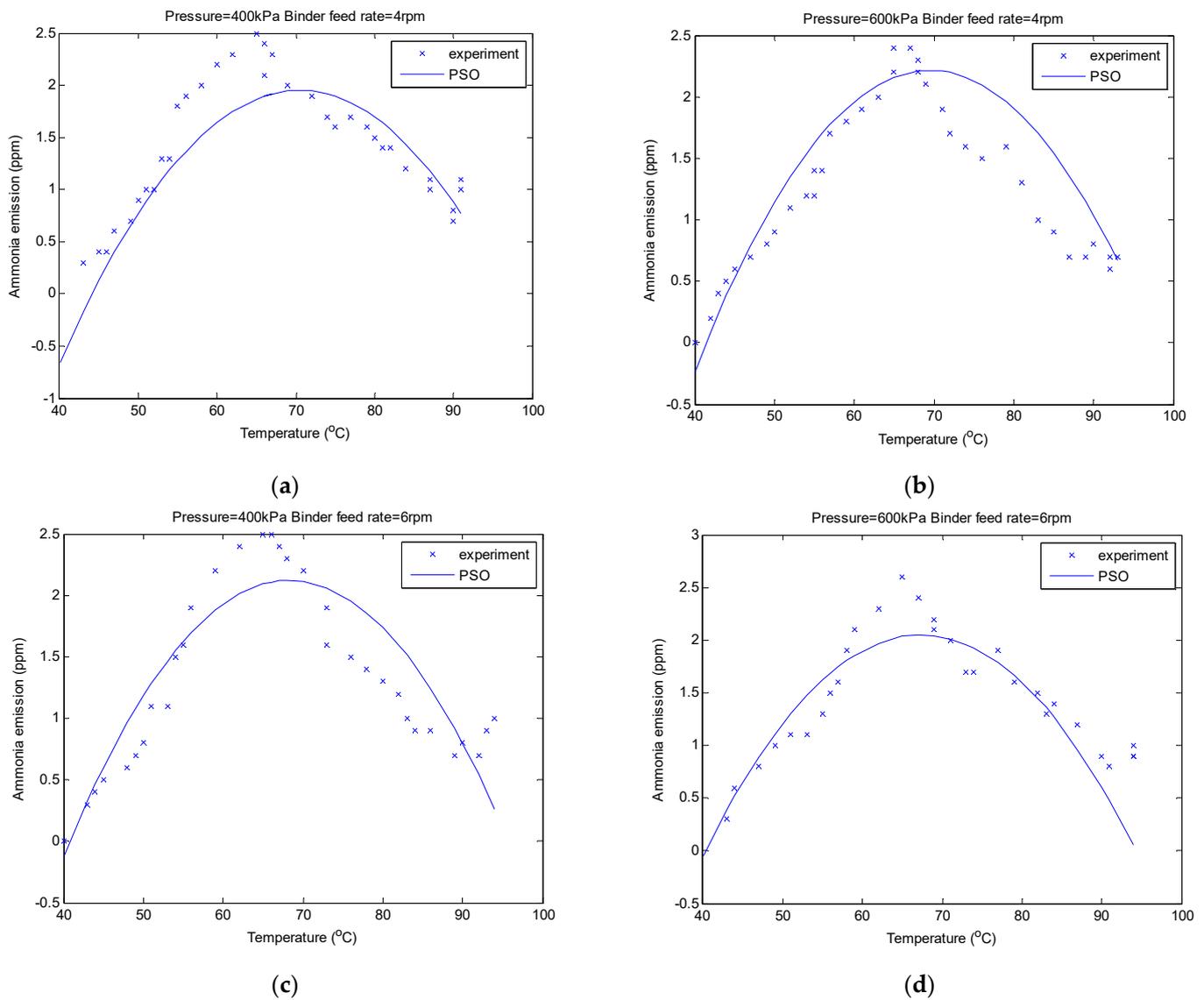
**Figure 5.** Ammonia emission predicted (PSO) and actual (experiment) vs. temperature over two different binder feed rates.



**Figure 6.** Ammonia emission predicted (PSO) and actual (experiment) vs. temperature over three different pressures.

Figure 7 shows a two-dimensional graph of the best model's predicted ammonia release in comparison with the actual value collected from the experiment for a clearer view

on the fitting of the quadratic model based on the optimized parameters. It can be seen that the model has a good fit for prediction of ammonia emission of less than 2 ppm. The error is higher for greater values of ammonia emission.



**Figure 7.** Ammonia emission predicted (PSO) and actual (experiment) vs. temperature over different pressure and feed rate settings (a) 400 kPa, 4 rpm (b) 600 kPa, 4 rpm, (c) 400 kPa, 6 rpm (d) 600 kPa, 6 rpm.

The swarm behavior can be observed via the convergence curve of the MSE vs. iteration in Figure 8. It is observed that both average and the best solution's MSE values gradually decrease. No premature convergence is observed. This is contributed by the chosen inertia weight. The decreasing inertia weight allows the swarm to balance between exploration and exploitation, which contributes towards minimizing the MSE efficiently.

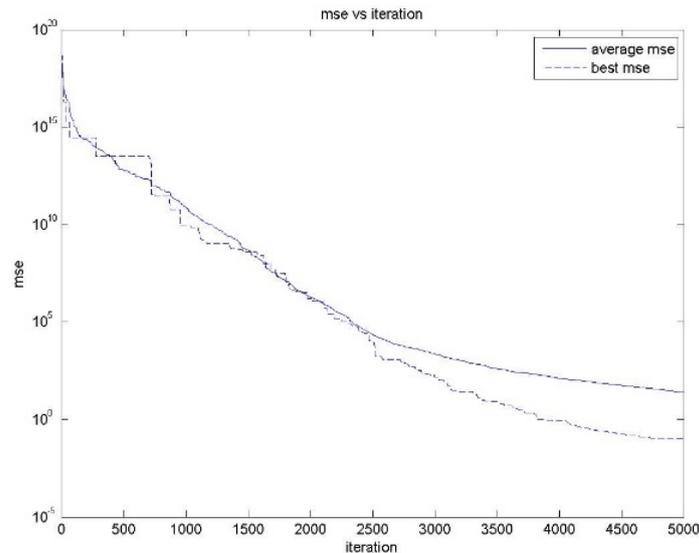


Figure 8. MSE vs. iteration.

## 6. Conclusions

PSO is employed in this research to optimize the model of the top-spray fluidized bed granulator. Three significant variables, namely binder feed rate, pressure and temperature, are selected for investigating the proposed optimization of the fluidized bed granulation model. The quadratic polynomial model is used for modeling and PSO is applied to search for the optimal coefficients. The optimized model performances are measured and validated using the MSE with respect to the actual experimental data. The best MSE is small and close to zero, 0.0973. Hence, it can be concluded that the developed model can be used to predict the minimum amount of ammonia gas released accurately with slight variation of the actual value.

The findings of this research show that PSO can be efficiently applied in designing an optimal mathematical model of a fertilizer's fluidized bed granulation system. The mathematical model can be used for improved, sustainable and healthy green manufacturing of bio-fertilizer. Specifically, the developed model enables sustainable production of the urea fertilizer with advanced parameter setting. The manufacturing with optimal parameter setting allows for fertilizer production with least ammonia emission and low risk of environmental pollution.

Based on the no-free lunch theorem, there is possibility that other optimization algorithms can solve this parameter optimization better than the PSO with linearly decreasing inertia applied here. Hence, in future studies, we will investigate the application of other optimization algorithms in solving this problem. Additionally, with more data, machine learning techniques such as artificial neural networks or regression can be considered alongside PSO to improve predictive capabilities. A dynamic model that considers temporal fluctuations, sensitivity analysis to identify crucial parameters and multi-objective optimization that takes into account things like production cost and the energy use could help to improve the system even more. Accounting for uncertainties, experimental validation and the use of sophisticated control methods such as model predictive control are to be considered for better sustainable manufacturing practice.

**Author Contributions:** N.M. and N.A.A.A. contributed to experimental design, analysis writing and editing. N.A.A.A., A.K.G. and M.R.S. contributed to validation, review, visualization and investigation. Project administration was prepared by N.M. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research is funded by the Ministry of Higher Education of Malaysia under the Fundamental Research Grant Scheme (FRGS/1/2012/TK06/MMU/03/7) and the Multimedia University IR Fund (MMUI/230034).

**Data Availability Statement:** The data utilized in this study can be accessed for research purposes by contacting the corresponding author.

**Acknowledgments:** We extend our gratitude to Multimedia University and Universiti Teknikal Malaysia Melaka for their support in facilitating this research.

**Conflicts of Interest:** The authors declare no conflicts of interest.

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