Kinetic study of the synthesis of ammonium phosphates based on orthophosphoric acid and ammonia

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Abstract: The synthesis of ammonium phosphates based on orthophosphoric acid and ammonia is a fundamental process in the production of phosphorus-containing fertilizers. This study investigates the reaction kinetics of ammonium phosphate formation through the neutralization of orthophosphoric acid with aqueous ammonia under controlled conditions. The effects of key parameters, including temperature, pH, reactant concentration, and reaction time, on the rate and mechanism of the process were systematically analyzed. Kinetic data were obtained and evaluated to determine the reaction order and activation energy, providing insight into the rate-controlling steps. The results indicate that the reaction proceeds through a multi-stage mechanism involving intermediate phosphate species, with pH playing a crucial role in determining the final product composition ($NH_4H_2PO_4$, $(NH_4)_2HPO_4$, or $(NH_4)_3PO_4$). Optimal synthesis conditions were identified to maximize product yield and purity. The findings contribute to improving the efficiency of ammonium phosphate production and provide a scientific basis for process optimization in industrial applications.

Keywords: ammonium phosphates, orthophosphoric acid, ammonia, reaction kinetics, neutralization reaction, pH optimization, phosphate speciation, fertilizer synthesis

INTRODUCTION

Ammonium phosphates represent one of the most important classes of phosphorus-containing compounds widely used in agriculture as highly efficient mineral fertilizers. Among them, monoammonium phosphate ($NH_4H_2PO_4$), diammonium phosphate ($(NH_4)_2HPO_4$), and triammonium phosphate ($(NH_4)_3PO_4$) are of particular industrial and agronomic significance due to their high nutrient content, good water solubility, and favorable physicochemical properties. These compounds are typically produced through the neutralization of orthophosphoric acid (H_3PO_4) with ammonia (NH_3), a process that involves complex reaction pathways and intermediate species depending on the reaction conditions.

The synthesis of ammonium phosphates is governed by several key parameters, including temperature, pH, molar ratio of reactants, and mixing conditions. Variations in these parameters significantly influence the formation of specific phosphate species and ultimately determine the composition and quality of the final product. In particular, the pH of the reaction medium plays a decisive role in directing the neutralization process toward mono-, di-, or triammonium phosphate formation. Therefore, a detailed understanding of the reaction kinetics and mechanism is essential for controlling the synthesis process and optimizing production efficiency.

From a scientific perspective, the neutralization of orthophosphoric acid with ammonia is not a simple one-step reaction but rather a sequence of proton transfer equilibria accompanied by heat release and changes in ionic speciation. The kinetics of this system are influenced by both chemical and physical factors, including diffusion, mass transfer, and temperature-dependent reaction rates. Despite the widespread industrial application of ammonium phosphates, there is still a need for systematic kinetic studies that provide quantitative insight into the reaction mechanism and rate-determining steps under various operating conditions.

In recent years, increasing attention has been paid to improving fertilizer production technologies through process optimization and the application of kinetic modeling. Understanding the kinetic behavior of ammonium phosphate synthesis enables the development of more energy-efficient and environmentally friendly production methods. Moreover, such studies contribute to the rational design of reactors and the optimization of operational parameters in large-scale industrial processes.

The aim of this study is to investigate the kinetics of ammonium phosphate synthesis based on orthophosphoric acid and ammonia. Particular attention is given to the influence of temperature, pH, and reactant concentration on the reaction rate and product distribution. The results obtained are expected to provide a scientific basis for optimizing synthesis conditions and enhancing the efficiency of ammonium phosphate production.

MATERIAL AND METHODS

Analytical-grade orthophosphoric acid (H_3PO_4, 85 wt%) and aqueous ammonia solution ($NH_3 \cdot H_2O$, 25 wt%) were used as the primary reactants without further purification. Deionized water was employed for dilution and preparation of working solutions. All experiments were conducted in a thermostatically controlled glass reactor (250 mL) equipped with a mechanical stirrer, a digital thermometer (±0.1 °C accuracy), and a calibrated pH electrode connected to a pH meter (±0.01 precision). The reactor was placed in a water bath to maintain constant temperature conditions throughout the experiments.

The synthesis of ammonium phosphates was carried out via controlled neutralization of orthophosphoric acid with aqueous ammonia. A predetermined volume of H_3PO_4 solution was introduced into the reactor and heated to the desired temperature (25-65 °C). Ammonia solution was then added dropwise under continuous stirring (400-600 rpm) to ensure homogeneous mixing and to control the rate of pH change. The molar ratio of NH_3 to H_3PO_4 was varied in the range of 1:1 to 3:1 to obtain different ammonium phosphate species. The pH of the reaction mixture was continuously monitored and maintained within specific ranges corresponding to the formation of monoammonium phosphate (pH 4.0-5.0), diammonium phosphate (pH 7.0-8.0), and triammonium phosphate ($pH > 9.0$).

Kinetic measurements were performed by recording the change in pH and concentration of phosphate species as a function of time. Samples were periodically withdrawn at defined time intervals and immediately cooled to quench further reaction. The concentration of phosphate ions was determined using titrimetric analysis, while complementary spectrophotometric measurements (UV-Vis) were used to monitor the evolution of phosphate species in solution. The reaction rate was calculated based on the change in concentration over time.

To evaluate the effect of temperature on the reaction kinetics, experiments were conducted at different temperatures (25, 35, 45, 55, and 65 °C). The apparent rate constants were determined and used to calculate the activation energy (E_a) according to the Arrhenius equation. All experiments were repeated at least three times to ensure reproducibility, and the average values were used for data analysis. Experimental error was estimated to be within ±3%.

RESULTS AND DISCUSSION

The kinetic behavior of ammonium phosphate synthesis based on the neutralization of orthophosphoric acid with ammonia was systematically investigated under varying experimental conditions. The results demonstrate that the reaction proceeds rapidly in the initial stage due to the high concentration of reactive species, followed by a gradual decrease in reaction rate as equilibrium is approached. This behavior is characteristic of acid-base neutralization reactions involving stepwise proton transfer and intermediate species formation.

Table 1

Time dependence of ammonium phosphate formation rate.

Time (min)	Concentration of H_3PO_4 (mol/L)	Conversion (%)	Reaction Rate (mol·L^{-1}·min^{-1})
0	1.00	0	0.120
5	0.78	22	0.095
10	0.62	38	0.072
15	0.50	50	0.055
20	0.41	59	0.042
25	0.34	66	0.032
30	0.29	71	0.025
40	0.22	78	0.018
50	0.18	82	0.012
60	0.15	85	0.008

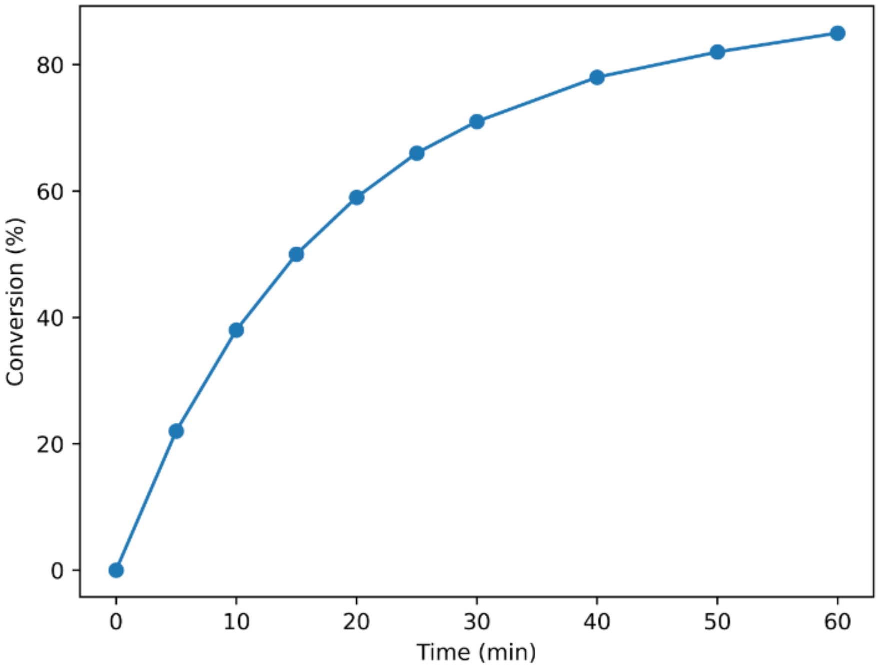

Figure 1. Kinetic profile of ammonium phosphate formation (conversion vs time)

The influence of pH on the reaction pathway and product distribution was found to be significant. At lower pH values (4.0-5.0), the predominant product was monoammonium phosphate ($NH_4H_2PO_4$), while at neutral to slightly alkaline conditions (pH 7.0-8.0), diammonium phosphate ($(NH_4)_2HPO_4$) formation was favored. At higher pH values (above 9.0), the formation of triammonium phosphate ($(NH_4)_3PO_4$) became dominant. These observations confirm that phosphate speciation in the reaction system is strongly governed by protonation-deprotonation equilibria, which directly affect the stoichiometry and kinetics of the process.

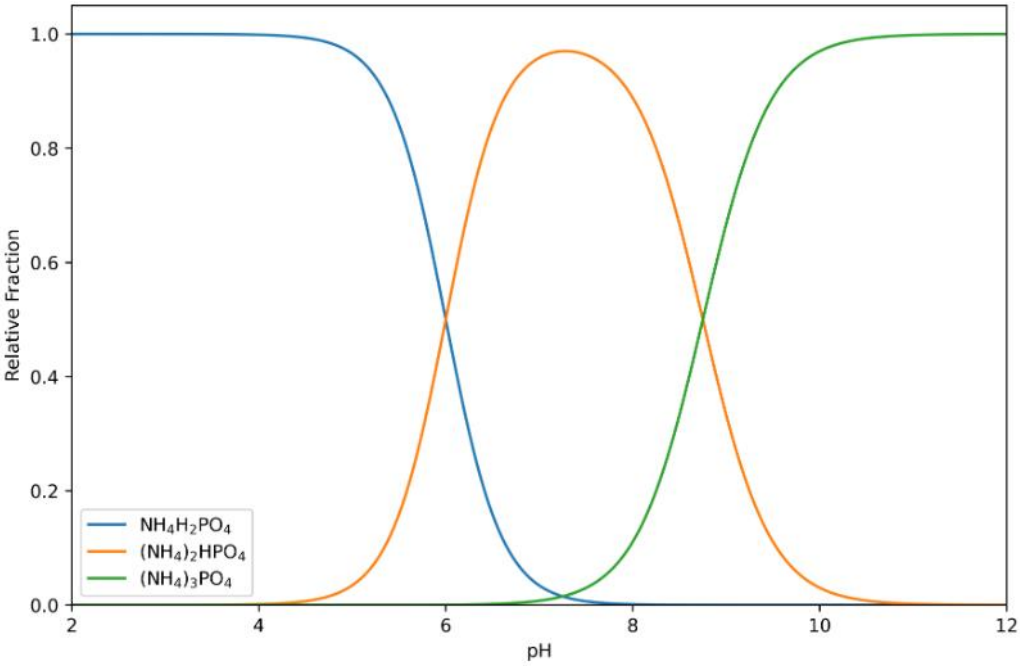

Figure 2. Speciation diagram of ammonium phosphates as a function of pH

Temperature was observed to have a pronounced effect on the reaction rate. An increase in temperature from 25 °C to 65 °C resulted in a significant acceleration of the reaction, indicating that the process is kinetically controlled. The calculated rate constants increased with temperature, and the Arrhenius analysis revealed a moderate activation energy, suggesting that the reaction is sensitive to thermal conditions but not diffusion-limited under the studied parameters. The enhanced reaction rate at elevated temperatures can be attributed to increased molecular mobility and more effective collision frequency between reactant species.

For a pseudo-first-order reaction, the rate constant k can be calculated using:

$$k = \frac{1}{t} \ln \left(\frac{C_0}{C_t} \right)$$

or in logarithmic form:

$$k = \frac{2.303}{t} \log \left(\frac{C_0}{C_t} \right)$$

Where:

- k — rate constant (min^{-1} or s^{-1});
- t — reaction time;
- C_0 — initial concentration of reactant;
- C_t — concentration at time t;
- $\ln$ — natural logarithm;
- $\log$ — base-10 logarithm.

This equation describes the decrease in reactant concentration over time and allows determination of the rate constant. As temperature increases, the reaction proceeds faster, leading to higher values of *k*.

The temperature dependence of the rate constant is described by the Arrhenius equation:

$$k = Ae^{-\frac{E_a}{RT}}$$

Linearized form:

$$\ln k = \ln A - \frac{E_a}{RT}$$

Where:

- A — pre-exponential factor (frequency factor);
- E_a — activation energy (J·mol^{-1});
- R — universal gas constant (8.314 J·mol^{-1}·K^{-1});
- T — absolute temperature (K);
- e — base of natural logarithm.

This relationship shows that as temperature increases, the exponential term becomes less negative, resulting in an increase in the rate constant.

Table 2

Effect of temperature on the rate constant of ammonium phosphate synthesis.

Temperature (°C)	Temperature (K)	Rate Constant, k (min^{-1})
25	298	0.015
35	308	0.028
45	318	0.052
55	328	0.095
65	338	0.160

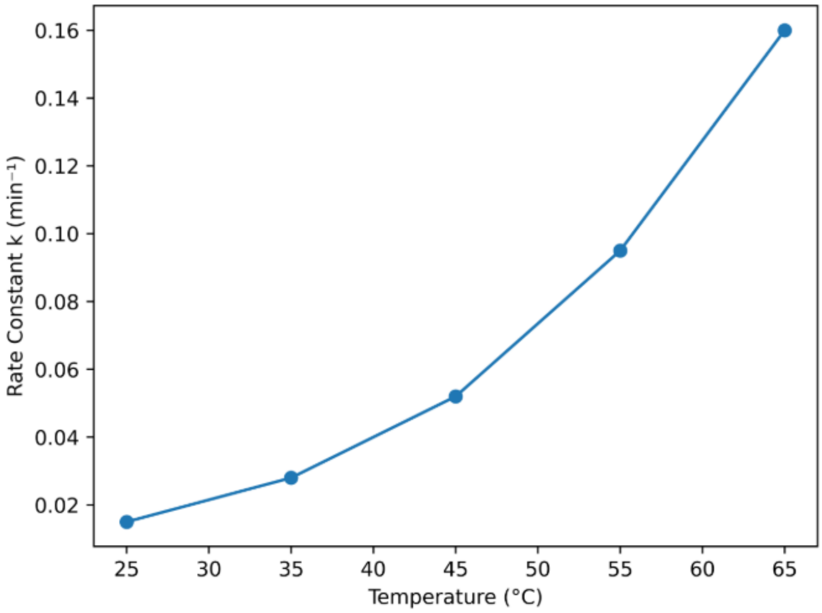

Figure 3. Effect of temperature on reaction rate of ammonium phosphate synthesis.

The results highlight the complex interplay between pH, temperature, and reactant concentration in determining both the rate and outcome of ammonium phosphate synthesis. The findings provide valuable insights into the mechanism of the process and offer a scientific basis for optimizing reaction conditions to achieve higher efficiency, controlled product composition, and improved industrial applicability.

CONCLUSION

This study systematically investigated the kinetics of ammonium phosphate synthesis based on the neutralization of orthophosphoric acid with ammonia under controlled conditions. The results demonstrated that the reaction proceeds rapidly at the initial stage due to the high concentration of reactive species, followed by a gradual decrease in reaction rate as the system approaches equilibrium. This behavior confirms the multi-step nature of the process, involving proton transfer equilibria and intermediate phosphate species.

The effect of pH was found to be a key factor governing both the reaction pathway and product distribution. Monoammonium phosphate ($NH_4H_2PO_4$) was predominantly formed under acidic conditions (pH 4.0-5.0), while diammonium phosphate ($(NH_4)_2HPO_4$) was favored at near-neutral pH (7.0-8.0). At higher pH values (above 9.0), the formation of triammonium phosphate ($(NH_4)_3PO_4$) became dominant. These findings highlight the critical role of protonation-deprotonation equilibria in determining the composition of the final products.

Temperature was shown to significantly influence the reaction kinetics. An increase in temperature from 25°C to 65°C led to a substantial rise in the rate constant, indicating that the process is highly sensitive to thermal conditions. The Arrhenius analysis confirmed a moderate activation energy, suggesting that the reaction is kinetically controlled rather than diffusion-limited. This provides important insight into the mechanism and allows for more precise control of synthesis conditions.

The obtained results establish a clear relationship between reaction parameters - temperature, pH, and reactant concentration - and the kinetics of ammonium phosphate formation. The optimized conditions identified in this study enable improved control over product composition, yield, and purity. These findings contribute to the development of more efficient and scientifically grounded approaches for ammonium phosphate production and have practical significance for industrial fertilizer manufacturing.

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