Numerical simulation for the formation of nanoparticles through vapor condensation in a reactor

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Abstract. The thermal plasma process is a highly efficient industrial method with many benefits. It works at high temperatures to make sure particles reach their vaporization point.. This numerical study, conducted using the Computational Fluid Dynamics (CFD) software ANSYS Fluent 2025R1, is significant as it aims to synthesize titanium alloy particles through condensation from the vapor phase, ultimately leading to the formation of nanoparticles. The study found that nucleation is affected by changes in plasma temperature. This, in turn, decreases the supersaturation ratio. It also emphasizes the need for careful control in the reactor environment to obtain a steady particle size distribution.

1 Introduction

The demand for nanoparticles on an industrial scale has increased due to their unique physical properties and applications across various sectors, such as electronics[1], pharmaceuticals[2], chemicals, and mechanical engineering [3]. This demand has led many researchers to create specific methods for producing these particulates, including mathematical and simulation techniques. The synthesis of nanoparticles has received significant attention. The synthesis of nanoparticles has gained considerable attention, prompting investigations into their properties and the effects they have on spherical particles.

Numerical studies on nanoparticles encounter challenges with both small and large particles. These challenges are influenced by condensation factors and the properties of their initial structures[2]. Understanding reactor models helps us see how particles form over time. This process depends on heat dissipation and the chemical interactions between the particles and the inert gas. The behavior of gas particles often needs turbulent reaction models to handle the transport equations involved. In plasma reactors, the flow of particles usually follows a non-linear pattern and changes with the distance traveled.

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The computational method for modeling turbulence has made it easier to use the probability density function (PDF) [3]to study the different physical properties of nanoparticles.

Particles first form through nucleation and then grow. Research on these processes has seen competition in the literature, with an emphasis on the structure and properties of the particles[4].

During the spheroidization process, particles transition through three phases depending on their size and thermodynamic properties as they pass through the plasma flame. First, the particulates become nanoparticles under critical vaporization conditions. Second, they take on a spherical shape once they reach their melting point. Finally, the yield particles look like their raw materials. This leads to a particle diameter that is larger than what we see during the melting phase. The principles behind these processes come from the uneven condensation of vapor onto gas particles. This offers helpful information about how the particles [5, 6]evolve.

The condensation process related to nanoparticles depends on the saturation conditions of the vapor. This outlines the main stage that leads to the formation of nuclei, which then grow. In this work, we develop a numerical model to help understand the condensation of injected titanium during the spheroidization process. The model examines the interactions influenced by plasma temperature and investigates the nucleation phase once supersaturation is achieved.

The formation of nanoparticles presents challenges in achieving the desired size and shape. It is essential to create an environment that encourages uniform nanoparticle formation. The flow setup can affect this process. One effective way to improve nanoparticles and find their size distribution is to use the quench gas. [7, 8]. In numerical studies, residence time also impacts the nanoparticles, including the heating interval along their paths, which affects their size distribution and the drag force experienced in the solid phase. The statistical methods used to describe the size distribution of nucleated particles and their condensation through vapor are influenced by the coagulation mechanism and processing timeframe [9].

Xiaoming Hao et al. [10] employed a Monte Carlo approach to simulate the growth of TiO2, integrating the population balance method within the aerosol reactor. The initial phase of nucleation is significantly affected by a substantial increase in gas temperature, which can hinder particle development during extended heating in the plasma region.

Recent developments have shown that both residence time and particle diameter are influenced by the carrier gas [11, 12]. However, there are relatively few adequate numerical studies investigating the interactions with material vapor, particularly in the case of titanium, which is often considered a pure substance. Analyzing this effect on the formed nuclei within a multicomponent gas-phase system is of particular interest.

This study aims to examine the influence of source temperature, evaporation rate, and inert gas pressure on the size and morphology of particles. Comprehending the reactor model will elucidate the mechanisms of particle formation. This emphasizes thermal dissipation and the chemical interactions between the particles and the inert gas.

2 Model and methods

2.1 Numerical simulations

The formation of titanium was implemented in the computational fluid dynamics (CFD) software, Ansys Fluent 2025R1, using a 3D model based on the x, y, z coordinate system. The model was analyzed in the x-y direction with uniform mesh Discretization. We used a pressure-based approach to solve the gas-phase equation (1), using second-order methods for

pressure, momentum, turbulence, and energy. The heat transfer and flow mechanisms that affect the size distribution of nanoparticles were based on our previous study[13].

$$\frac{\partial(\rho\emptyset)}{\partial t} + \nabla \cdot (\rho u\emptyset) = \nabla \cdot (\Gamma_\phi \nabla\emptyset) + \dot{S}_\emptyset + \dot{S}_{\emptyset,p} \tag{1}$$

where ρ is the fluid density, u is the velocity vector of the fluid, $\emptyset$ and s is the scalar quantity, Γ_ϕ Is the diffusivity and $\dot{S}_\emptyset$ is the source term.

2.2 General dynamic equation

The concentration number of nanoparticles at the k node is calculated using the general dynamics equation (GDE) [14], which is expressed as follows:

$$\frac{dN(k)}{dt} = \frac{dN(k)}{dt}\bigg|_{\text{nucl}} + \frac{dN(k)}{dt}\bigg|_{\text{coag}} + \frac{dN(k)}{dt}\bigg|_{\text{evap/cond}} \tag{2}$$

where $N(k)$ is the rate of concentration of nucleation, coagulation, and evaporation. The rate of coagulation is assumed to be negligible in this work, because it is believed that the coalition of particles of small sizes is modest, and the equation is reduced to the following:

$$\frac{dN(k)}{dt} = \frac{dN(k)}{dt}\bigg|_{\text{nucl}} + \frac{dN(k)}{dt}\bigg|_{\text{evap/cond}} \tag{3}$$

2.3 Synthesis of titanium nanoparticles

The synthesis of titanium nanoparticles is governed by the nucleation rate and is influenced by the evaporation of titanium Particles in the plasma region. In the numerical simulation, we modeled the evaporation behavior for this process using a user-defined function based on the supersaturation ratio (S). This ratio shows when the vapor becomes saturated (for S > 1). This saturation leads to nucleation, where new nuclei form within the reactor. This ratio shows when the vapor becomes saturated (for S > 1). This saturation leads to nucleation, where new nuclei form within the reactor chamber after condensation. The supersaturation ratio is a critical parameter for nanoparticle synthesis and nucleation, defined as the actual partial pressure of the vapor over the equilibrium saturation pressure of the particle at a given temperature.

$$S = \frac{p}{p_s(T)} \tag{4}$$

where S is the supersaturation ratio, p is the partial pressure of the monomer, and p_s is the saturation vapor pressure, expressed as a function of temperature according to the following equation(5) for the titanium material [15]:

$$Log\, \boldsymbol{p}_s = 7.782 - \left(\frac{24275}{T}\right) - 0.230 \times 10^{-3}T \tag{5}$$

If the supersaturation condition is satisfied (S > 1), the saturation concentration n_s It can be defined as the ratio of the saturation vapor pressure. Consequently, the product of the Boltzmann constant k_B And the temperature can be expressed as follows:

$$n_s = \frac{p_s}{k_B T} \tag{6}$$

The nucleation process becomes valid when the supersaturation condition is met, leading to the formation of particles at a critical radius. This is essential for calculating the conversion of gas to particle nucleation, expressed as[16]:

$$r^* = \frac{2\sigma v_1}{k_B T(\ln S)} \tag{7}$$

It is important to note that the nucleation process is sensitive to temperature changes in the plasma. These variations can significantly affect the critical diameter of the nuclei and the nucleation rate. The critical Gibbs free energy barrier for the formation of the nucleus, once the melting point is reached, is given by:

$$\Delta G^* = \frac{16\pi\sigma^3 v_m^2}{3(K_B T)^2 (lnS)^2} \tag{8}$$

The classical nucleation rate (CNT) of the formed particles is described as follows [18]:

$$J = J^* \exp\left(-\frac{\Delta G^*}{K_B T}\right) \tag{9}$$

Where J^* is the approximate pre-exponential factor [17]. σ is(*10*) the surface tension of the material, v_m^2 is the molar volume of the monomer, K_B is the Boltzmann constant (1.38e-23 J/K), and T is the temperature.
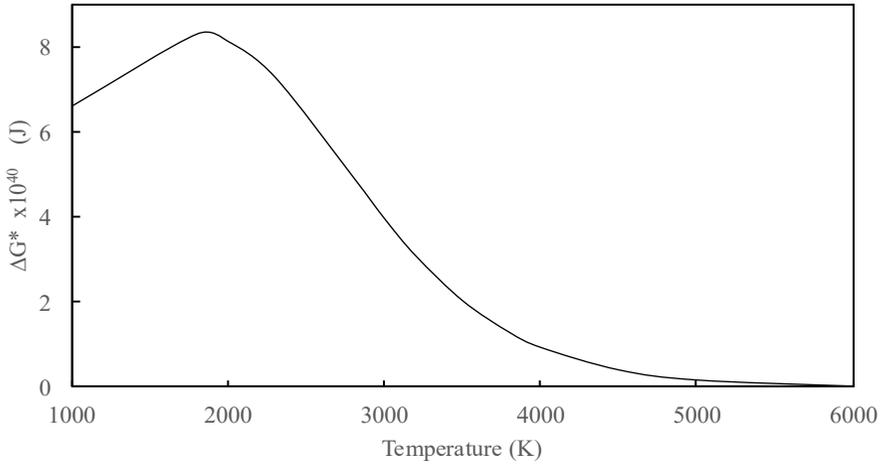
Fig. 1. Gibbs energy barrier for titanium in argon gas as a function of temperature.

The kinetic theory during nanoparticle synthesis describes how vapor molecules collide to form critical particles. A key factor influencing the size distribution of particles and their growth dynamics in the vapor phase is the nucleation rate, represented.

$$J^* = \frac{P_v x_v}{k_B T} \sqrt{\frac{2\sigma}{\pi m}}$$

(10)

where P_v and x_v Denote the partial pressure and mole fraction of titanium gas, respectively, and \(m\) is the mass of titanium. The overall nucleation rate can be derived by combining equations (9) and (10).

$$J = \frac{P_v x_v}{k_B T} \sqrt{\frac{2\sigma}{\pi m}} \exp\left[\frac{16\pi\sigma^3 v_m^2}{3(K_B T)^3 (lnS)^2}\right]$$

(11)

A C-code was developed and compiled to simulate particle behavior using the Lagrangian approach, as denoted in the Discrete Phase Model (DPM). In this model, particles are tracked individually with each computational cell. The phenomenon of evaporation is defined by equation (12), conditioned by the saturation vapor pressure of titanium, which is proportional to gas temperature. The mass evaporation rate is modeled (*13*)by:

$$E_r = E_c * (T - T_{melt})$$

(12)

To more precisely simulate the phase transitions, the simulation considered spatial and temporal fluctuations in temperature and pressure inside the chamber. And the mass of the evaporated particles with the time step resulted in the following equation:

$$dm = E_r * dt \tag{13}$$

3 Results and discussion

Titanium particles spheroidized at 1941 K at the melting temperature, which results in the formation of spherical particles; however, they become partially vaporized when these particles reach boiling temperature, causing supersaturation on their surface, resulting in metal vapor formation via homogeneous nucleation and the formation of nanoparticles.

In the CFD model, equations (5) to (13) were considered as user-defined scalars, written as a source of code in the C language. The numerical studies took place in a model built with Fluent software, whose plasma torch and reactor were 50x200 and 370x1100 mm, respectively. The whole dimension of the model is found in our previous work [13]. Argon gas was used as the main gas, and titanium as the material.
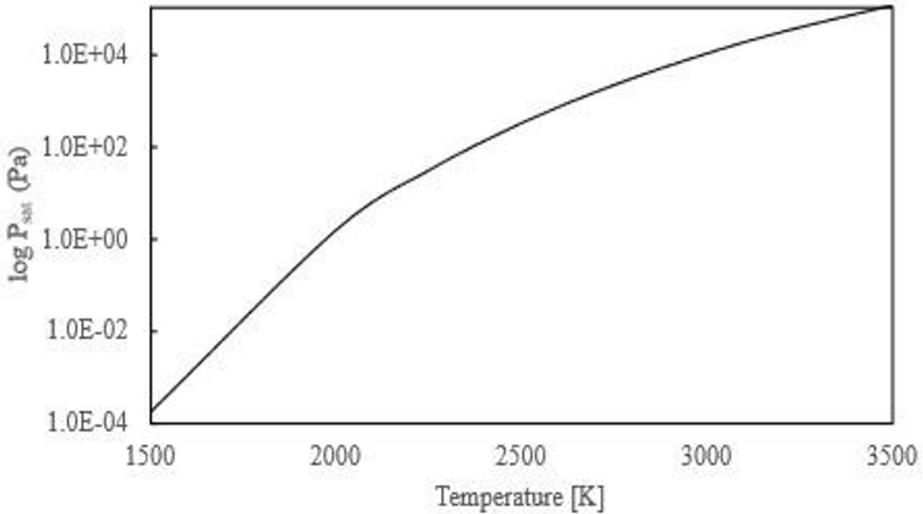

Fig. 2. Distribution of saturation vapor pressure as a function of temperature displayed on a logarithmic scale.
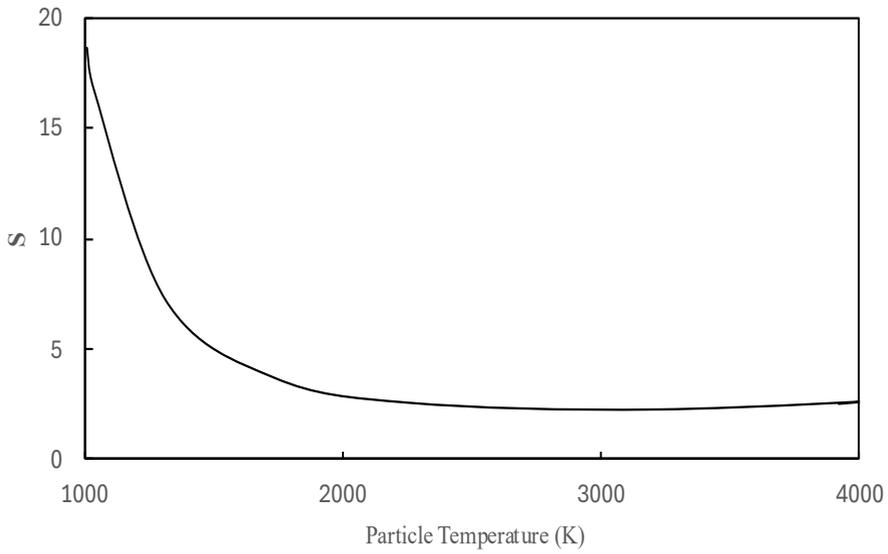
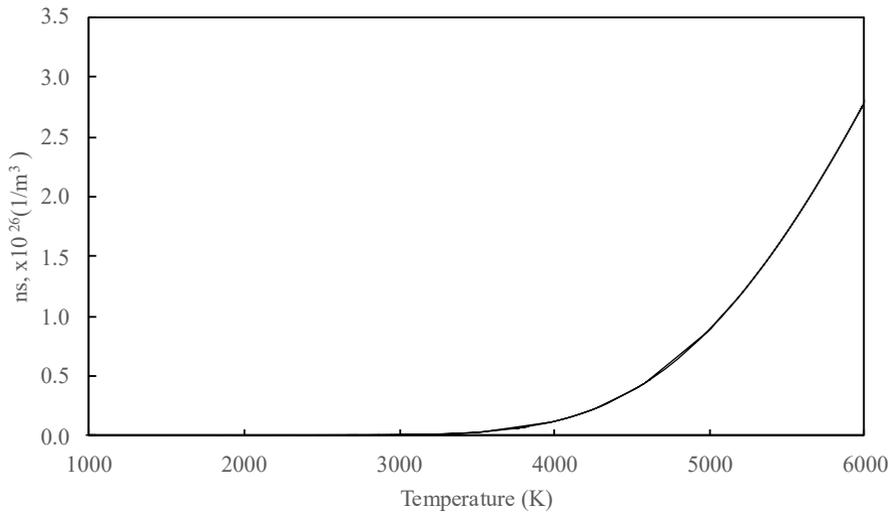**Fig. 3.** The variation of saturation ratio as a function of temperature distribution

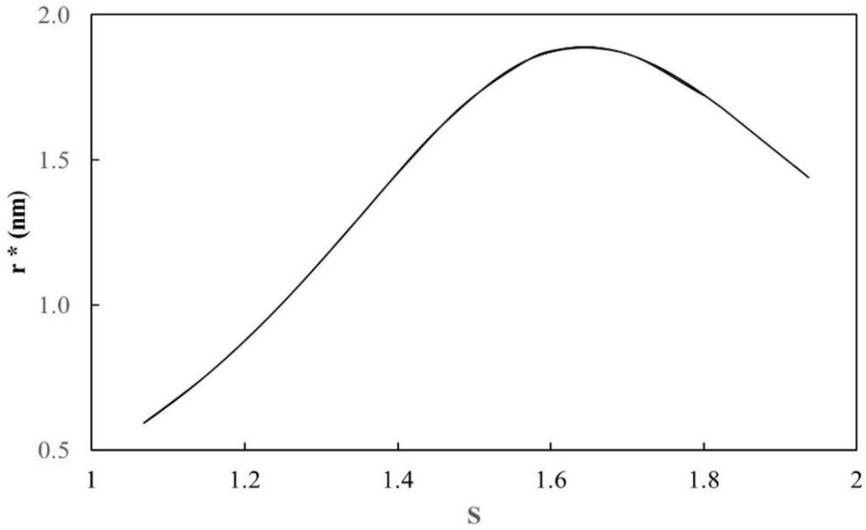**Fig. 4**. The temperature dependence of titanium vapor saturation concentration.

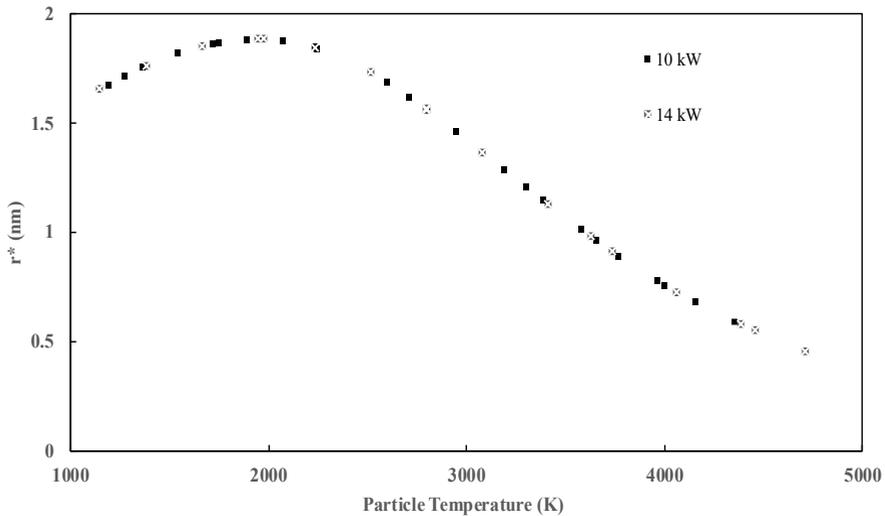**Fig. 5.** Saturation impact on the critical radius of the formed nuclei.

Fig. 6. Energy input impact on critical radius defined at 10 and 14 kW as source term.

The temperature gradient significantly influences the saturation vapor pressure (see Fig. 2) and, consequently, the supersaturation ratio (see Fig. 3). Both factors are crucial for the formation of nanoparticles. As the temperature increases, the supersaturation ratio (S) decreases, which reduces the thermodynamic driving force for nucleation. In areas with higher temperatures, titanium vaporizes more, leading to an increased vapor flux. However, this often halts particle growth and results in smaller particles. This observation is consistent with previous reports on the production of nanoparticles in the vapor phase. Initially, titanium particles form as the saturation concentration rises (**Fig. *4***)[18]. This occurs because titanium vaporizes and then nucleates. However, as the temperature increases, the importance of the saturation vapor pressure also rises, effectively lowering the supersaturation, even when nucleation events are still occurring.

When the gas temperature exceeds titanium's melting point, as shown in Fig. 1, the nucleation energy barrier decreases further, accelerating particle formation. However, this process can also lead to the formation of unstable nuclei that are subject to evaporation or growth. This phenomenon has been observed in studies of high-temperature condensation of refractory metals. The critical nucleus radius reaches its maximum at higher gas temperatures (see Fig. 6). As the flow cools and the vapor condenses towards the exit of the chamber, the critical nucleus radius decreases. These findings are consistent with classical nucleation theory and support previous studies suggesting that temperature affects nucleation kinetics and establishes a balance between growth and evaporation, thereby influencing the size distribution of the particles.
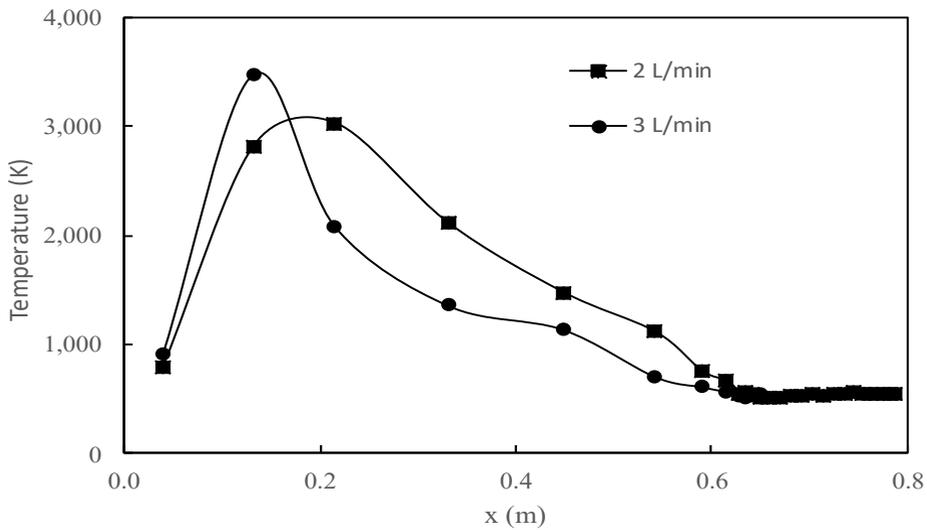

Fig. 7. Effect of carrier gas on titanium material.

Fig. 7 illustrates the impact of the argon carrier gas. As the flow increases, the average critical radius tends to increase, leading to the formation of particles. This is mainly due to the decreasing residence time of vapor species in the reactor, which restricts the duration for adequate supersaturation to occur, thereby decreasing the nucleation rate. Increasing the argon flow rate from 2 to 3 L/min results in an observed temperature drop of roughly 14%. This decrease in temperature can improve condensation by inducing nucleation, thus increasing the mass of the condensed phase. However, if residence time is not managed correctly with the quenching gas, larger particles may continue to evaporate beyond the ideal condensation zone, lowering the overall particle yield.
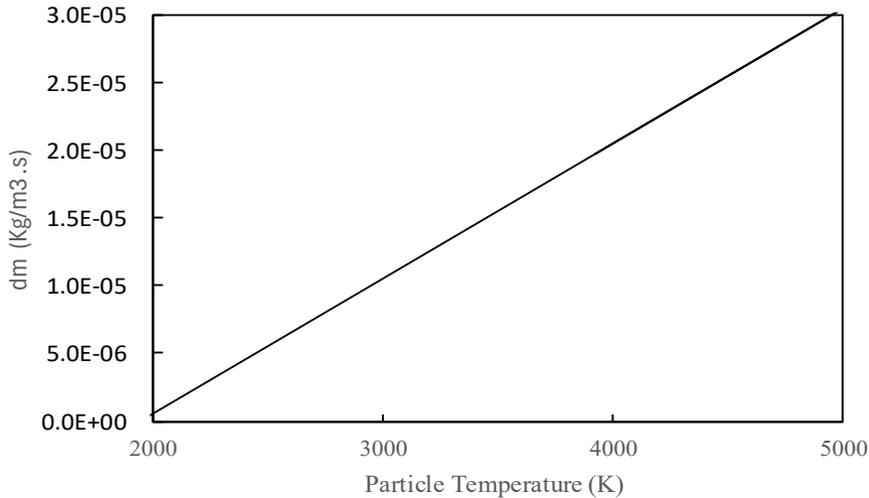
Fig. 8. Effect of the mass evaporation of particles along their trajectories in the plasma reactor.

Fig. 8 shows a linear increase in mass loss with an increase in temperature. This visualizes a small amount of mass evaporating. It is essential to adjust the residence time and temperature to control the formation of nanoparticles. Moreover, avoid massive vaporization that creates instability for condensation to occur, as seen in Fig. 5. That demonstrates the effect of the supersaturation ratio on the stability of the formed nuclei. This is due to temperature dependency on the surface area[19]. Therefore, it is observed that the critical radius deviates from the ideal gas effect on the mixing, and nucleation tends to be difficult.

4 Conclusion

The study focuses on the formation of titanium nanoparticles. It was found that the nucleation process is susceptible to changes in temperature, residence time, and supersaturation ratio. On the other hand, it was observed that the plasma temperature and the carrier gas greatly influenced the particle size distribution and the critical radius of the formed nuclei. Nucleation can be enhanced by increasing the flow of the carrier gas, as it facilitates a more effective cooling process; however, when the flow rate is increased, it impacts the residence time, which is not advantageous for larger particles. This paper enlightens the advantages of controlling different factors to optimize the production of nanoparticles. These outcomes highlight the means for controlling nanoparticle formation in high plasma medium and guide further validation of an experimental process.

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