

Modeling the Heating Rate Dependent Size Evolution of Iron Oxide Nanoparticles in Thermal Decomposition Method

Project report submitted to Visvesvaraya National Institute of Technology, Nagpur in partial fulfillment of the requirements for the award of the degree

Bachelor of Technology

In

Chemical Engineering

By

Pratik P. Patil (BT18CME041)

under the guidance of

Dr. C. Ravi Kumar



Department of Chemical Engineering

Visvesvaraya National Institute of Technology

Nagpur 440 010 (India)

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Declaration

I, Pratik Prakashrao Patil, hereby declare that this project work titled, “**Modeling the Heating rate Dependent size evolution of Iron Oxide Nanoparticles in Thermal Decomposition Method**” is carried out by me in the Department of Chemical Engineering of Visvesvaraya National Institute of Technology, Nagpur. The work is original and has not been submitted earlier whole or in part for the award of any degree/diploma at this or any other Institution / University.

Date:

Sr.No	Enrollment No	Name	Signature
1	BT18CME041	Pratik P. Patil	

Certificate

This is to certify that the project titled “**Modeling the Heating rate Dependent size evolution of Iron Oxide Nanoparticles in Thermal Decomposition Method**”, submitted by ‘Pratik P. Patil (BT18CME041)’ in partial fulfillment of the requirements for the award of the degree of **Bachelor of Technology in Engineering, VNIT Nagpur.** The work is comprehensive, complete and fit for final evaluation.

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ABSTRACT

We studied modeling the heating rate dependent size evolution of iron oxide nanoparticle in thermal decomposition method. To obtain the insights of the nucleation and growth of iron oxide nanoparticle we simulated the model equations. The simulation results replicate the experimental data, and they are well fitted to the well-known LaMer model that is depicted by the burst of nucleation and the separation of nucleation and growth under constant monomer supply condition.

We studied the influence of heating rate on crystal growth, size, and monodispersity of iron oxide nanoparticles. By implementing classical nucleation theory and theoretical growth model, we recognized the heating rate and precursor-to-monomer conversion rate as a key factor inducing the final size and dispersity of the nanoparticles.

By modeling the heating rate various parameters were simulated to understand the Iron Oxide Nanoparticle formation and to understand how the evolution takes place.

The parameters such as Supersaturation, particle size distribution, nucleation rate, heating rate were simulated and studied. The variation of different parameters at different heating rate and were useful in understanding the particle formation and its evolution. By performing simulation we were able to find out the various heating rate impact on the final iron oxide nanoparticle size.

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CHAPTER 1. INTRODUCTION

1.1 Iron Oxide Nanoparticle

Iron oxide nanoparticles are iron oxide particles with a diameter of 1 to 100 nanometers[1]. Magnetite (Fe_2O_3) and its oxidised variant maghemite ($\gamma\text{-Fe}_2\text{O}_3$) are the two most common forms. They've sparked a lot of attention because of their superparamagnetic properties and potential applications in a variety of fields.

Iron oxide nanoparticles are one of the most intriguing materials right now, not just because of their fundamental scientific importance, but also because of their many technical uses, including permanent magnets, recording media, and biomedical diagnosis and therapy. The precise control of nanoparticle size and a small size distribution are essential for achieving highly sensitive nanoparticles.

1.2 Structure of Magnetite

Magnetite has an inverse spinel structure. The oxygen in magnetite forms a face-centered cubic crystal framework. In magnetite, all the tetrahedral sites are occupied by Fe^{2+} and octahedral sites are occupied by both Fe^{3+} and Fe^{2+} . Maghemite is distinguished from magnetite by the presence of cation vacancies in the octahedral sites and that all or most of the iron in the trivalent state (Fe^{3+}) [2].

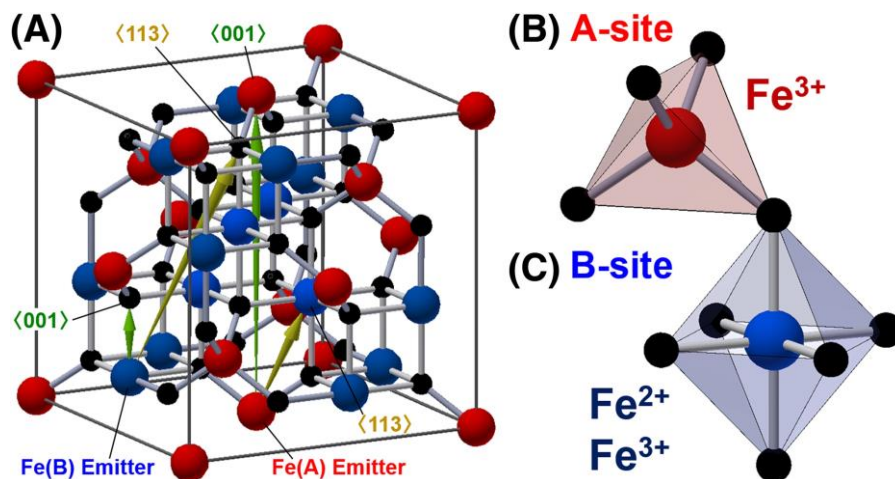


Fig 1: Structure of Magnetite[3]

Ref:- Site-sensitive X-ray photoelectron spectroscopy of Fe_3O_4 by photoelectron diffraction; By:-Yusuke Hashimoto et.al.

1.3 Applications of Iron Oxide Nanoparticles

Magnetic NPs have attracted much interest as a labeling material in life sciences and various other major fields of the scientific world. Iron oxide NPs because of their strong magnetic properties were used first in biology and then in medicine for the magnetic separation of biological products and cells, as well as for site-specific drug delivery. The surface chemistry, size, and charge of magnetic particles influence biodistribution of the NPs. Activities in the clinical applications, in the past decades, of magnetic carriers and particles are increasing due to their role in diagnostics and treatment modalities. [3]

Biomedical:- Magnetic NPs coated with liposomes are used for drug delivery, magnetic hyperthermia, MRI contrast agent, magnetic separation, controlled drug release, cellular therapy, like cell labeling, tissue repair, cell separation and handling of cells, purifying cell populations, magnetofection, diseases of the musculoskeletal system, severe inflammation, disability, and pain.[3]

Health care:- Therapeutic targets in chemotherapy (cancer and tumor), nanoscale biosensors and imaging, nanocoatings on surfaces, implant, nanocarrier for vaccination, antimicrobial activities, in drug delivery and research, nano photothermolysis with pulsed lasers for the treatment of cancer, hepatitis B virus, respiratory syncytial virus, influenza virus, antiviral agents against HIV-1, monkeypox virus, herpes simplex virus type 1, and Tacaribe virus; delivering antigens for a particular disease into the bloodstream; preventing aging of the skin[3].

Agriculture and food:- Nano-based products like nanofertilizers, nano-fungicides, nanopesticides, engineered NPs, and CNTs boost crop yields; for seed treatment for various plants prior to sowing the seeds, pyrite NPs are used which results in broader leaf morphology, larger leaf numbers, increased biomass and enhanced breakdown of stored starch. This has increased the possibility of developing iron pyrite NPs as a commercial seed treatment agent as a pro-fertilizer, as the process does not put NPs into the soil; this is a safe strategy. It reduces dose requirement as compared to chemical fertilizers and no adverse effects on plant growth. Nanosensors, nanofood, encapsulation, food packing, nanocoatings, precision farming (remote-sensing devices), nanocomposites, gene transfer (crop improvement), and nanoporous membranes.[3]

Environmental remediation:- For pollution prevention used for detection, monitoring, and remediation; used in permeable reactive barriers, membrane filtration, adsorption for wastewater treatment. For carbon capturing used in artificial leaf for CO₂ sequestration, mineral carbonation, biomimetic carbonation, N₂O decomposition, methane combustion. Improves manufacturing processes (efficiency, waste reduction), dematerialization (reduction in material quantity), sensing (pollutant sensors, nanoporous membranes, chemical and bio-nanosensors, nanowire sensor for explosives), and energy (heat distribution, eg, ceramic-like materials that provide sufficient reliability and durability of the entire structure)[3].

Energy:- Photovoltaic film coatings, improved efficiency of fuel production and consumption, fuel cells and batteries, nanobioengineering of enzymes, thermoelectric materials, and prototype solar panels, batteries, aerogels, conversion of waste heat in computers, automobiles, homes, power plants, etc, to usable electrical power[3].

Defense and aerospace:- Nanocomposites, nanocoatings, sensors and electronics, fuel additives and energy devices, and smart materials[3].

Construction:- Nanocoatings, nanocomposites, nanoscale sensors, smart materials, and additives to concrete. Iron oxide pigments are used in coloring concrete, brick, tile, and other construction materials[3].

Automotive :- Used as additives in catalysts and lubricants, nanocoatings, fuel cells, composite fillers, and smart material[3].

Textiles:- Sensors, nanofibers, coatings, and smart materials[3].

Electronics:- Printed electronics, carbon nanotubes, nanoscale memory, nanowires, NEMS, spintronics, and quantum dots[3].

1.4 Synthesis of Iron Oxide Nanoparticle

There are many methods for synthesising Iron oxide nanoparticles:-

1.4.1 Coprecipitation

Coprecipitation from aqueous solutions is a simple and most frequently used method and allows the preparation of magnetic NPs with rigorous control of size and shape. The reaction of Fe(II) salt, in aqueous solution, to a base in the presence of mild oxidant synthesizes spherical NP of 30–100 nm. The factors on which the phase and size of the particles depend are the concentration of cations, the presence of counter ions, and pH of the solution. NPs by coprecipitation usually aggregate because of large surface-area-to-volume ratio and to reduce surface energy. To stabilize, dispersing agents are added to stabilize them like anionic surfactant, can also be achieved by coating the surface with proteins, starches, nonionic detergents, or polyelectrolytes as the adsorption of such substances stabilizes the electrolyte concentrations of particles that would otherwise be high enough[3].

1.4.2 Microemulsion

Water-in-oil micro-emulsion have nanosized water droplets dispersed in the oil phase. The droplets are stabilized by surfactant molecules. The nanocavities lemmatize particle growth, nucleation, and agglomeration. The diversity of NPs due to surfactant, nature, physiological conditions, etc, is the main advantage of this technology. For the synthesis of magnetite NPs, nanoemulsion containing iron source and sodium hydroxide are mixed together, later lysed with acetone to remove the surfactant and washed with ethanol. Normally, the colloidal NPs exhibit superparamagnetic behavior with high magnetization values.

There are several dissolved components in the water and oil phase; therefore, the selection of the surfactant (and cosurfactant) depends upon the physicochemical characteristics of the system. Different surfactants, such as cationic, anionic, or nonionic, can be used. The main disadvantage associated with this method is adverse effects of residual surfactants on the properties and difficulty in scale-up procedures.

1.4.3 Sol-gel Method

This method revolves around hydroxylation and condensation of molecular precursors in solution. Obtained “sol” from nanometric particles is then dried or “gelled” either by solvent removal or by chemical reaction to obtain a three-dimensional metal oxide network. The solvent used is water, but the precursors can be hydrolyzed using an acid or a base. Basic catalysis yields a colloidal gel, whereas acid catalysis formulates a polymeric gel. The reaction is performed at room temperature; however, heat treatment is required to obtain the final crystalline state. shows the reaction mechanism of magnetite particle formation from an aqueous iron(III) solution by sol–gel system.

Disproportionation : $\text{Fe}^{3+} + \text{H}_2\text{OFe}(\text{OH})_x^{3-x}$

Oxidation : $\text{Fe}(\text{OH})_x^{3-x}$

Magnetite dehydration : Fe_3O_4 (pH 9.0, 60 °C)

1.4.4 Gas/aerosol phase methods

For continuous, high, and direct production of defined magnetic NPs, spray and laser pyrolysis is an efficient technique. A solution of ferric salts is sprayed into the reactor in the presence of reducing agents. The solute condenses while the solvent evaporates. Later, the dried residue consisting of particles is obtained, whose size is the same as the original. Maghemite particles from 5 nm to 60 nm with diverse shapes have been generated using different iron precursors.

1.4.5 Polyols method

Polyols method is a significant technique for the preparation of well-defined NPs with controlled shape and size. After controlling the kinetics of the precipitation, non-agglomerated metal particles with well-defined shape and size can be obtained. The average size of the metal particles is controlled by reactive medium, heterogeneous nucleation. The synthesis steps are independent of resulting uniform particle size. Iron NPs of 100 nm can be obtained by ferrous hydroxide in organic media. The solvents used, such as polyols and polyethylene glycol, offer interesting properties due to their high dielectric constants. These solvents can dissolve inorganic compounds, and due to their relatively high boiling points they offer a wide operating temperature range.

1.4.6 Hydrothermal reaction methods

The hydrothermal reactions are performed in a reactor or autoclave in an aqueous media, where the conditions are maintained at pressure of more than 2,000 psi and temperature of more than 200°C. The dehydration of metal salts and low solubility of oxides in aqueous phase supersaturate the medium. The size and shape are greatly affected by temperature, precursor, and the time on morphology and particle size, precursor concentration, residence time[3].

1.4.7 Sonolysis

IONP can be synthesized by the decomposition/sonolysis of organometallic precursors by adding metal chloride with Metaloxides(NaOH), then they decompose or sonolysed using Ultrasonic irradiation. As capping agents or structural hosts polymers are used, to limit the growth of the NPs. Ultrasonic irradiation causes cavitation in an aqueous medium, where the formation, growth, and collapse of microbubbles occur and yields amorphous NPs.

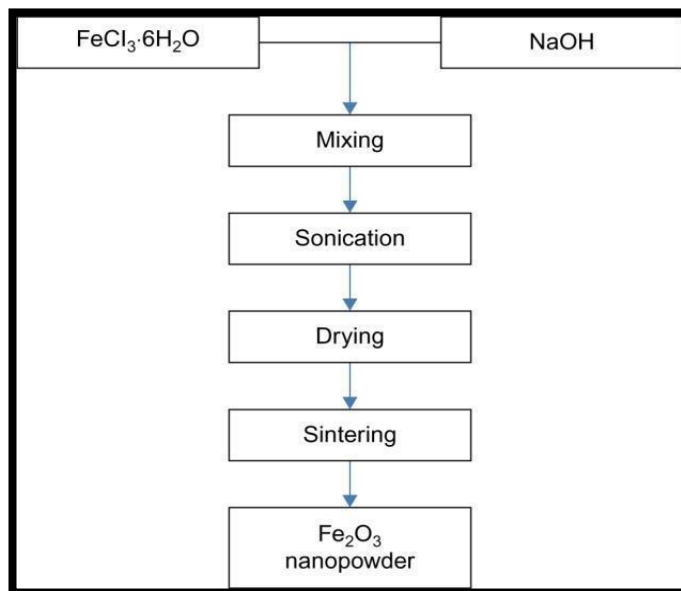


Fig 2: Sonolysis synthesis of IONP

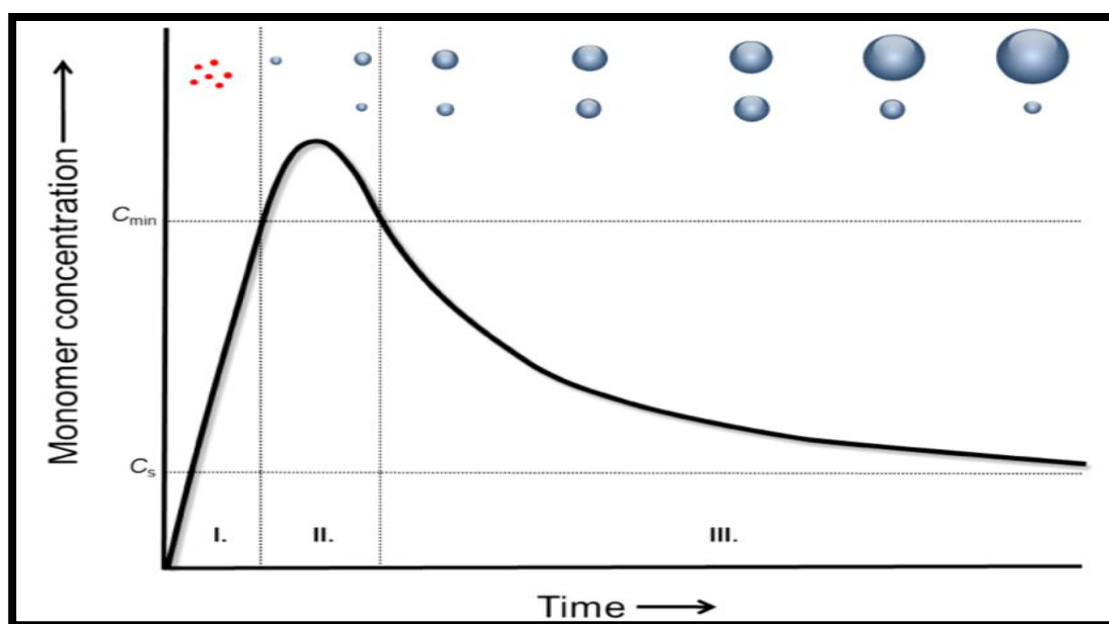
Ref;- Systematic Review of the Preparation Techniques of Iron Oxide Magnetic Nanoparticles ;By:- S. F. Hasany, I. Ahmed, Rajan J, A. Rehman

1.4.8 Thermal Decomposition

It is a kind of sonolysis in which Thermal or heat is given to the system and a certain temperature is maintained for the system of metal oleate complex/organometallic complex and solvent to obtain IONP. IONP obtained are crystalline and size and shape varies as the temperature, concentration of precursors, surfactant, aging time, heating rate and environment of the system. We will be focusing on Thermal Decomposition for further processing as it gives crystalline IONP and we will try to determine how size depends on the factors affecting.[4]

1.4 LaMer Theory

One of the classic models for synthesis of Nanoparticles is proposed by LaMer in which the nuclei are allowed to slowly diffuse, resulting in growth, until the final size is attained. In order to attain mono disparity, nucleation should be avoided during the period of growth. So nucleation starts when saturation is achieved and then nucleation and growth happens simultaneously.



Ref:- Enhanced Nanoparticle Size Control by Extending LaMer's Mechanism ; By:- Erika C. Vreeland,† John Watt,† Gretchen B. Schober.

Fig. 3: LaMer Theory (closed system), stage I: Increase in concentration of free monomer till saturation, Stage II :- Reach saturation concentration and nucleation takes place then decrease in conc. Of monomer. Stage III :- Growth of Nucleus with decrease in concentration of precursor or monomer for further growth of NP.

CHAPTER 2 -THERMAL DECOMPOSITION METHOD

2.1 Synthesis of Thermal Decomposition of IONP

The Thermal Decomposition's procedure starts by making metal oleate complex by reacting metal chlorides and sodium oleate . The iron–oleate complex is prepared by reacting iron chloride ($\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$) and sodium oleate. The iron chloride and sodium oleate is dissolved in a mixture solvent composed of ethanol, distilled water and hexane. The resulting solution is heated to $70\text{ }^\circ\text{C}$ and kept at that temperature for four hours.

When the reaction is completed, the upper organic layer containing the iron–oleate complex is washed three times with distilled water in a separatory funnel. After washing, hexane is evaporated off and results in iron–oleate complex in a waxy solid form.

The iron-oleate complex synthesized as described above with oleic acid (surfactant) are dissolved in 1-octadecene (solvent) at room temperature. The reaction mixture is heated to $320\text{ }^\circ\text{C}$ with a constant heating rate of $3.3\text{ }^\circ\text{C min}^{-1}$ (can be varied), and then kept at that temperature for 30 min. When the reaction temperature reaches $320\text{ }^\circ\text{C}$, a severe reaction occurs and the initial transparent solution becomes turbid and brownish black. The resulting solution containing the nanocrystals is cooled to room temperature, and ethanol is added to the solution to precipitate the nanocrystals. The nanocrystals can be separated by centrifugation [5].

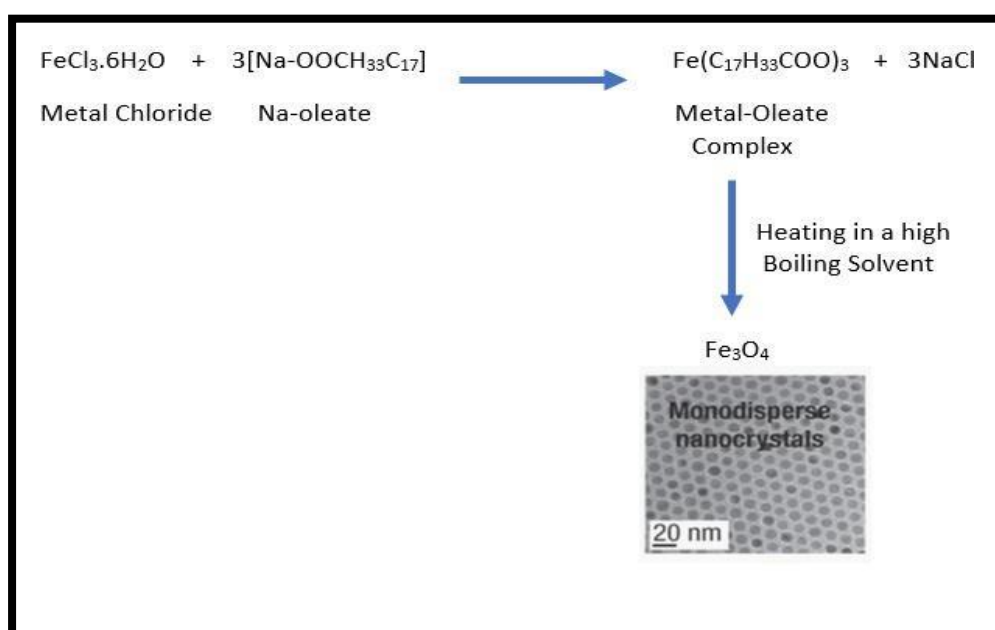


Fig 4: Thermal Decomposition Procedure.

Ref:- Synthesis, functionalization, and nanomedical applications of functional magnetic nanoparticles ; By:Zhou Chen et.al.

2.2 Factors influencing the Size of iron oxide nanoparticles

2.2.1 Temperature:- The formation of nucleus of IONP happens in a system at a certain temperature only. The data was summarized for the system containing below is the table of the formation of IONP when the system was at different temperatures.[6]

Table 1: Nuclei formation and size of IONP at different temperatures[5]:

Summarizing the variation with temperature.

Temperature	Aging time	Conclusions
310°C	-	No nanoparticle formation
320°C	-	Uniform nanoparticles size ranging from 8nm to 11nm
320°C	10,20,30 min	Monodisperse 12 nm nanocrystals.
260°C	1 day	Polydisperse & poorly crystalline 9nm nanoparticles.
260°C	3 days	Monodisperse 12 nm nanocrystals
240°C	1 day	No NP
240°C	3 days	Highly polydisperse 14nm particles
200°C	3 days	No NP were formed

According to the literature survey and study it was found that at low temperature NP were not formed i.e around 200⁰C, at 240⁰C IONP needs aging time for formation

where as at temperature greater than 300⁰C IONP are formed around 320⁰C. If temperature is less then required aging time is more, at higher temperature aging time is less. But still the exact temperature of nucleation is not that well defined because there are discrepancies regarding nucleating temperature as there were many observations also when the solution color changed from red-brown to black and change in color of solution is a major indicator for IONP formation.

As according to LaMer theory separating nucleation and growth is necessary and Brownstein has stated that nucleation and growth are separated by 20⁰C. Increasing temperature gives shape variation at 360⁰C, spherical and at 380⁰C, cubic IONP were obtained.

2.2.2 Aging Time:- It is the time for which the system is maintained at a certain temperature to promote the growth of IONP nuclei i.e. to increase size. Again considering table 1 it is evident that more the aging time more will be size. But formation of nuclei is important before aging because if no nuclei there will be nothing to grow (take case at 200⁰C where 3 days aging was done still no IONP were formed).

Aging is important because there are cases where even the nuclei were observed only after some aging time even though the solution color was changed.

2.2.3 Precursor Concentration:- With increase in precursor concentration the size of NP increases, it is the same as high reaction concentration favours formation of product. Even LaMer theory in extended form said that keeping the reaction system open and continuous supply of precursor aid the growth of NP.

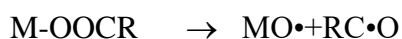
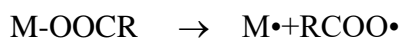
2.2.4 Heating Rate:- Separation of growth and separation is necessary for monodisperse NP formation. With a high heating rate the growth phase/ temperature will be reached soon but the nucleation is yet to start there is more possibility of overlapping the nucleation and growth phase causing polydisperse formation of NP rather than monodisperse it is even possible that no NPs are formed. Optimum heating rate is required to maintain separation between nucleation and growth.

CHAPTER 3. MODELING AND SIMULATION

3.1 Thermal Decomposition of Iron-Oleate Complex.

The decomposition reaction occurs through formation of thermal free radical.

When the M-O and MO-C bonds of a metal carboxylate break, radical species occur .



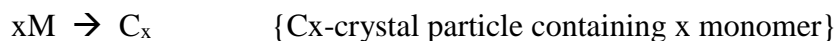
To propagate the decomposition reaction, these radical species can recombine, decompose into smaller molecules, or react with other metal carboxylate molecules.

3.2 Theoretical model for the synthesis of the nanocrystals

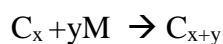
Process 1 (prenucleation stage)



Process 2 (nucleation stage)



Process 3 (growth stage)



In Process 3 supersaturation $S = [\text{M}] / [\text{M}]_{\text{eq}}$

{ $[\text{M}]_{\text{eq}}$ -Monomer concentration in equilibrium }

3.3 Modeling Equations

3.3.1 Standard Population Balance Model

$$\frac{\partial N(r,t)}{\partial t} + \frac{\partial [N(r,t) \Gamma(r,t)]}{\partial r} = R_{nuc} g(r)$$

Where

$N(r,t)$ is Number of particle of radius r at time t ,

$\Gamma(r, t)$ is the instantaneous growth rate,

R_{nuc} is the nucleation rate,

$g(r)$ is the nucleation distribution function.

3.3.2 Nucleation Rate

$$R_{nuc} = 8\pi r_m D N_A S^{pu+1} [C]_{\infty}^2 \exp\left\{ \frac{-(4\pi r_c^2 \gamma)}{3K_B T} \right\}$$

D - monomer diffusion coefficient

N_A - Avogadro constant

S - The dimensionless supersaturation defined as the bulk concentration of the monomer normalized to equilibrium concentration of the monomers.

Exponents of the supersaturation are the normalized critical radius to the monomer radius,

$$p = (r_c/r_m)^3$$

u - coagulation parameter

surface energy γ normalized to the thermal energy $K_B T$.

3.3.3 Nucleation Distribution Function $g(r)$

$$g(r) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(\frac{-k(r-r_c)^2}{2\sigma^2}\right)$$

$$k = 1 \text{ kJ mol}^{-1} \text{ nm}^{-1}$$

$$\sigma^2 = K_B T / 2$$

3.3.4 Instantaneous Growth Rate of a Particle

$$\Gamma(r,t) = \frac{dr}{dt} = \frac{D V m S (1 - \exp(2\gamma m / r R T))}{(r + \frac{D}{K_r})}$$

D -Monomer diffusion coefficient

γ - Surface Energy

K_r - Reaction rate

3.3.5 The Dynamics of the Precursor Release

$$\frac{d[P]}{dt} - \frac{-d[C]}{dt} = -A \exp(-E_A/RT)[P]$$

A - prefactor

E_A - precursor to monomer activation energy

3.3.6 Generalized Equation for the Supersaturation

$$S(t_{i+1}) = S(t_i) - Q \int_0^\infty dr r^3 \{n(r, t_{i+1}) - n(r, t_i)\} + \frac{A[P]\Delta t}{[C]_\infty} e^{\frac{-E_A}{RT}}$$

$$Q = \frac{4\pi\rho}{3M_W V_{tot}[C]_\infty}$$

$n(r, t_i)$ – number density of particles

M_W - monomeric molecular weight

V_{tot} - Volume of solution

E_A - Activation Energy

3.3.7 Heating Rate

$$\frac{dT}{dt} = H_R \quad \text{for } T \leq T_f$$

T_f - final temperature

H_R - heating rate

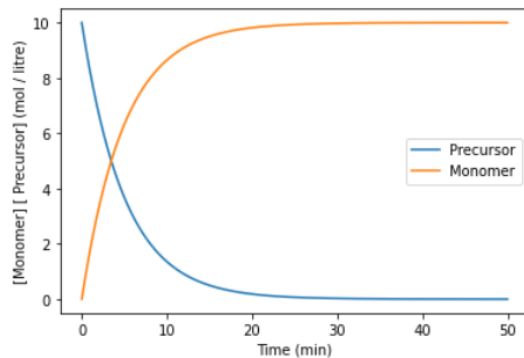
CHAPTER 4. SIMULATION CODE AND RESULTS

4.1 Variation of Precursor and Monomer during decomposition of the reaction

```
In [21]: import numpy as np
import matplotlib.pyplot as plt

t=np.arange(0,50,0.011)
y1=10*np.exp(-0.2*t)
y2=10*(1-np.exp(-0.2*t))
plt.plot(t,y1)
plt.plot(t,y2)
plt.xlabel('Time (min)')
plt.ylabel('[Monomer] [ Precursor] (mol / litre)')
plt.legend(['Precursor','Monomer'])
```

Out[21]: <matplotlib.legend.Legend at 0x180adfe4610>

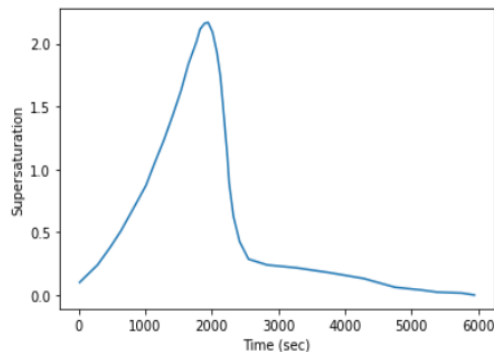


4.2. Supersaturation vs time (H_R-1.5K/min)

```
In [105]: import pandas as pd
import matplotlib.pyplot as plt

df = pd.read_excel (r'C:\Users\91845\Desktop\Plots project\book2.xlsx')
df=df.iloc[: , :6]
x=df['time']
y=df['S']
plt.plot(x,y)
plt.xlabel('Time (sec)')
plt.ylabel('Supersaturation')
```

Out[105]: Text(0, 0.5, 'Supersaturation')



4.3. Variation in size vs time

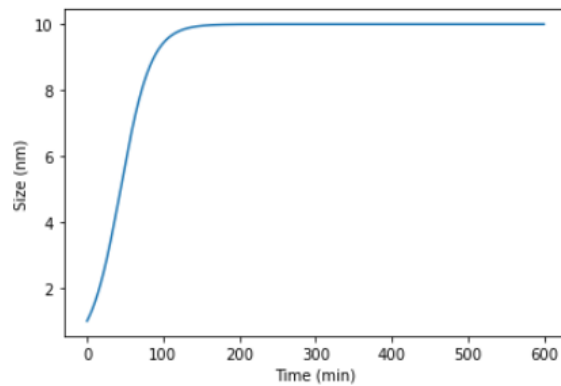
```
In [24]: import numpy as np
import matplotlib
matplotlib.use('tkagg')
import matplotlib.pyplot as plt
from scipy.integrate import odeint

y0 = [1] # start with 1 cell
t = np.linspace(0,600,num=1000)
r = 0.05
K = 10
params = [r,K]
def sim(variables,t,params):

    X = variables[0]
    r = params[0]
    K = params[1]
    dXdt = r*X * (1 - X/K)

    return([dXdt])
y = odeint(sim,y0, t, args=(params,))

plt.plot(t,y[:,0])
plt.xlabel("Time (min)")
plt.ylabel("Size (nm)")
plt.show()
```

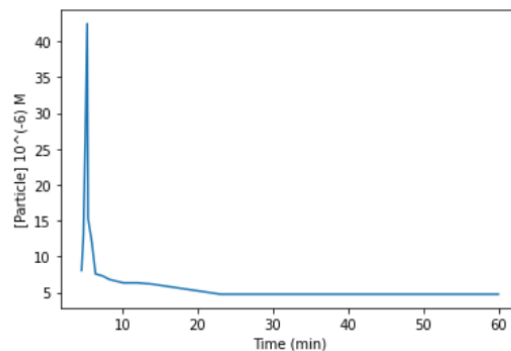


4.4 Particle Concentration vs time

```
In [112]: import pandas as pd
import matplotlib.pyplot as plt

df = pd.read_excel (r'C:\Users\91845\Desktop\Plots project\Nvstime.xlsx')
df=df.iloc[:, :6]
x=df['time']
y=df['N']
plt.plot(x,y)
plt.xlabel('Time (min)')
plt.ylabel('[Particle] 10^(-6) M')
```

Out[112]: Text(0, 0.5, '[Particle] 10^{^(-6)} M')



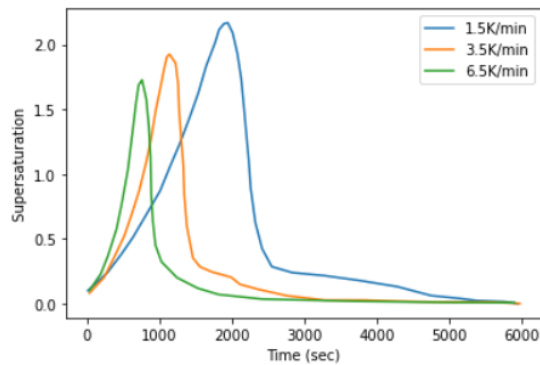
4.5 Supersaturation vs time

```
In [5]: import pandas as pd
import matplotlib.pyplot as plt

df = pd.read_excel(r'C:\Users\91845\Desktop\Plots project\book2.xlsx')
df=df.iloc[:, :6]
x1=df['time_1']
y1=df['S_1']
x3=df['time_3']
y3=df['S_3']
x6=df['time_6']
y6=df['S_6']
plt.plot(x1,y1)
plt.plot(x3,y3)
plt.plot(x6,y6)

plt.xlabel('Time (sec)')
plt.ylabel('Supersaturation ')
plt.legend(['1.5K/min', '3.5K/min', '6.5K/min'])
```

Out[5]: <matplotlib.legend.Legend at 0x214f314adc0>

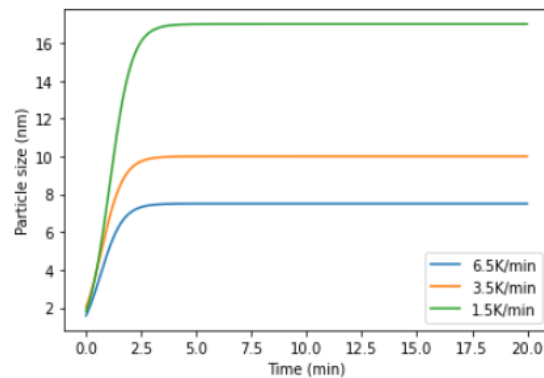


4.6 Radius vs time

```
In [7]: import numpy as np
import matplotlib.pyplot as plt

t=np.arange(0,20,0.011)
y1=7.5/(1+3.75*np.exp(-2*t))
y2=10/(1+4*np.exp(-2*t))
y3=17/(1+8.5*np.exp(-2*t))
plt.plot(t,y1)
plt.plot(t,y2)
plt.plot(t,y3)
plt.xlabel('Time (min)')
plt.ylabel('Particle size (nm)')
plt.legend(['6.5K/min', '3.5K/min', '1.5K/min'])
```

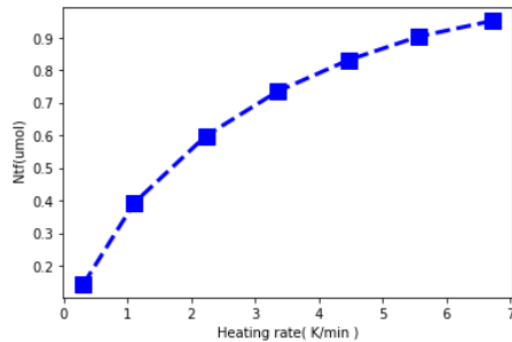
Out[7]: <matplotlib.legend.Legend at 0x2e7e9fa8fd0>



4.7 Number of NPs at the end of simulation vs heating rate

```
In [98]: import pandas as pd
import matplotlib.pyplot as plt
df = pd.read_excel(r'C:\Users\91845\Desktop\Plots project\Ntf vs Hr.xlsx')
df=df.iloc[:, :6]
x=df['Heating rate( K/min )']
y=df['Ntf(umol)']
plt.plot(x, y, color='b', linestyle='dashed', linewidth = 3,
         marker='s', markerfacecolor='blue', markersize=12)
plt.xlabel('Heating rate( K/min )')
plt.ylabel(' Ntf(umol)')
```

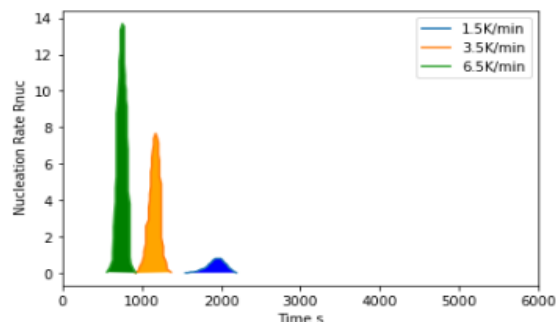
Out[98]: Text(0, 0.5, ' Ntf(umol)')



4.8 Nucleation Rate vs time

```
In [82]: import pandas as pd
import matplotlib.pyplot as plt
df = pd.read_excel(r'C:\Users\91845\Desktop\Plots project\Rnuc vs time.xlsx')
df=df.iloc[:, :6]
x_6=df['time_6.5K'].fillna(-1)
y_6=df['Rnuc_6.5K'].fillna(-1)
x_3=df['time_3.5K'].fillna(-1)
y_3=df['Rnuc_3.5K'].fillna(-1)
x_1=df['time_1.5K'].fillna(-1)
y_1=df['Rnuc_1.5K'].fillna(-1)
x_1=[i for i in x_1 if i>-1]
y_1=[i for i in y_1 if i>-1]
x_3=[i for i in x_3 if i>-1]
y_3=[i for i in y_3 if i>-1]
x_3.sort()
x_6=[i for i in x_6 if i>-1]
y_6=[i for i in y_6 if i>-1]
x_6.sort()
plt.plot(x_1,y_1)
plt.plot(x_3,y_3)
plt.plot(x_6,y_6)
plt.xlim([0,6000])
plt.xlabel('Time s')
plt.ylabel(' Nucleation Rate Rnuc')
plt.legend(['1.5K/min', '3.5K/min', '6.5K/min'])
plt.fill(x_1, y_1, "b")
plt.fill(x_3, y_3, "orange")
plt.fill(x_6, y_6, "green")
```

Out[82]: [<matplotlib.patches.Polygon at 0x2c4cd5421f0>]



5. CONCLUSION

We concluded that heating rate has a huge impact on the nucleation and the growth of the particle. We understood the factors influencing the particle formation. We understood the formation and the evolution of the iron oxide nanoparticle by simulating the model equation. The heating rate has an impact on the nucleation the evolution of the nanoparticle. When different heating rate was used we get the different particle size distribution. The saturation was impacted with different heating rate. The total number of particles at the end of the simulation was affected by the heating rate. As the heating rate was increasing the total final number of particles were increasing. The simulated model replicates the experimental trends and it was seen that the relative time scales related with the heating and precursor-to-monomer conversion rates is a key factor impacting the NP final size in thermal decomposition synthesis method. By simulation we can predict the final size of the nanoparticle at different heating rate.

6. **REFERENCES**

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- [2] Hamed Sharifi Dehsari et. al. ; Combined Experimental and Theoretical Investigation of Heating Rate on Growth of Iron Oxide Nanoparticles
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