Investigation of Temperature and Influent Load on Nitrifying Treatment of Using Wastewater CFD

Baharak Sajjadi, Mostafa Keshavarz Moraveji and Reza Davarnejad

Department of Chemical Engineering, Faculty of Engineering, Arak University, Arak 38156-8-8349, Iran

Abstract: The paper describes the effect of temperature, ammonia concentration and feed flow rate on nitrifying treatment of wastewater usage Computational Fluid Dynamics (CFD) for two phase bubbly flow in a split cylindrical airlift reactor with a 0.085 m initiator diameter and 0.505 m height. Superficial gas velocity was used as the operational parameter, air was used as the dispersed phase and wastewater containing ammonia was used as continuous phase. Temperature enhancement in a constant O₂ and NH₄⁺ concentrations, resulted the increase of reactions rate also NO₃⁻ had an increase of about 3 times as much. By the feed flow rate increase, O₂ consumption increase and the rate of NO₃⁻ production increase more than NO₂⁻ but decrease the reactions efficiency decrease in a constant time. NH₄⁺ concentration enhancement leads to the increase of O₂ consumption and better reactions efficiency at higher NH₄⁺ concentration, NO₃⁻ concentration increases more. Modeling results are compared with the experimental data. The CFD modeling results show suitable agreement with the experimental data.

Key words: Airlift reactor · Wastewater treatment · Nitrification · Free ammonia

INTRODUCTION

The world that we all live in and its development of technology and the industries, has created some problems in spite of making our lives more comfortable such as pollutions in soil, in water even in the air. Ammonia, nitrite and nitrate are some of the most harmful and common water pollutants which exist in many wastewaters. By injecting such wastewater to the environment running water and in continue to the cities piped water system, such material will be imported to human body. Gastric bacteria change the nitrite to nitrate and so influence on the digestion system, especially in children, in addition nitrite in stomach react with the amines, amides and produce nitroamine which will result gastric cancer after a long time [1-3].

In the environment running water ammonia ions are combined with oxygen and produce toxic materials, so oxygen concentration decreases and toxic material, increase which intimidate the aquatic life [4].

There are different methods for ammonia removal from wastewater, including physical-chemical processes, using filters, resins or osmosis methods and biological processes, but biological processes have a better efficiency and in a large scale, are more efficient economically so are investigated in many studies [2, 5]. Conventional biological nitrogen removal has two steps (nitrification and denitrification) that carry out subsequently or simultaneously, but this process is just useful for a low ammonia concentration and needs two separate reactors, but lately new processes have been studied and used, such as ANAMMOX, SHARON, CANON, OLAND and so on, that are more efficient and just need one reactor, because they contain one slight nitrification step to nitrite and nitrite tures to nitrogen gas, so the nitrite change to nitrate doesn't happen and the amount of oxygen consumption decreases and they are useful in wastewater with high amount of ammonia or combined with nitrogen [6-10].

In these processes, setting the optimum conditions are so important to decrease costs and time, but to increase efficiency. Simulation is one of the best methods for finding optimum parameters.

Corresponding Author: Mostafa Keshavarz Moraveji, Department of Chemical Engineering, Faculty of Engineering, Arak University, Arak 38156-8-8349, Iran. Tel: +98-9363098063, Fax: +98-861-4173450, E-mail: m-moraveji@araku.ac.ir.
Airlift bioreactors are one of the best equipments for two or three phase contacting. These reactors are characterized by many advantages such as suitable mixing without any movable section, closer contact between the phases, faster oxygen transfer rate, shorter reaction time and greater process capability. Changing and controlling the parameters are so easy in such reactors so they are suitable for biological processing like ammonia removal [11-12]. Several researchers have studied the hydrodynamics and mass transfer of nitrifying in bioreactors.

The influences of the bed (settled) volume on bioreactor volume ratio in a three-phase flow multiple airlift loop bioreactor, superficial air velocity Ua, hydraulic residence time HRT and pH value on ammonia nitrogen reduction were investigated by Jianping et al. [1].

Kouakoua et al. has developed a novel circulating a jet-loop submerged biofilm bioreactor (JLMBR) adapted to ammonium partial oxidation [13]. This study is intended to determine how gas–liquid mass transfer is affected by operating conditions, in order to obtain a high biomass retention time and to achieve a separate control of mixing and aeration they have adopted membrane technology is adopted and air and water forced circulation are combined.

The effects of temperature and free ammonia of landfill leachate on nitrification and nitrite accumulation were investigated by Kim et al. [14] with a semi-pilot scale biofilm airlift reactor they have found High free ammonia inhibited both from nitrite oxidizing bacteria (NOB) and also ammonia oxidizing bacteria (AOB).

Kim et al. have developed a sequencing batch airlift reactor (SBAR) to selectively enrich ammonia oxidizers as the dominant nitrifying bacteria and granulate ammonia oxidizers from wastewater nitrification [15]. Partial nitrification and reduced settling time were the selection pressures for the selective enrichment and granulation of ammonia oxidizers. They also achieved stable partial nitrification to accumulate nitrite.

Mosquera-Corrall et al. have studied effects of acetate and different salts present in feed of a SHARON reactor on partial nitrification of ammonia to nitrite the results indicate that the decrease in ammonia oxidizing activity was due to a competition for substrates between both heterotrophs and autotrophs bacteria [3].

Kempen et al. have constructed a SHARON system; they have found that due to the high ammonium influent concentrations pH control is of great importance and during a stable process, they removed 90% of N-ions via the nitrite route [16].

Astrid et al. have investigated, an autotrophic, synthetic medium for the enrichment of anaerobic ammonium-oxidizing (Anammox) microorganisms and they have shown acetylene, phosphate and oxygen to be strong inhibitors of Anammox activity [17].

Astrid et al. in another work have examined the Anammox process in detail. They have explained that the rate of ammonium oxidation was proportional to the initial amount of oxidizing sludge, also in addition chloramphenicol, ampicillin, 2,4-dinitrophenol, carbonyl cyanide m-chlorophenyl hydrazone and mercuric chloride completely inhibited the activity of the ammonium oxidizing sludge [18].

Jetten et al. have suggested the combination of two processes (anammox and Sharon) [19] and Dijkmen et al. have suggested the Cannon process using nitrite as an autotrophic for the first time and has had successful results [20].

The aim of the present study was to investigate the turbulence temperature, ammonia concentration and feed flow rate on nitrifying treatment of wastewater. CFD software was applied for this investigation.

**Problem Definition**

**Conventional Nitrification and Denitrification:**

Conventional microbial nitrogen removal is based on autotrophic nitrification and heterotrophic denitrification. Conversion of NH₄⁺ to NO₂⁻ and further to NO₃⁻, with oxygen molecules as the electron acceptor, is called nitrification. The relevant reactions are as follow:

\[
\text{NH}_4^+ + 1.5O_2 \rightarrow \text{NO}_2^- + 2H^+ + 2H_2O 
\tag{1}
\]

\[
\text{NO}_2^- + 0.5O_2 \rightarrow \text{NO}_3^- 
\tag{2}
\]

The anoxic denitrification (conversion of NO₂⁻ and NO₃⁻ to nitrogen gaseous) is accomplished with a variety of electron donors, including methanol, acetate, ethanol, lactate and glucose. The anoxic denitrification involves the following reactions [21]:

\[
2\text{NO}_2^- + 10H^+ + 10e^- \rightarrow N_2 + 2OH^- + 4H_2O 
\tag{3}
\]

\[
2\text{NO}_3^- + 6H^+ + 6e^- \rightarrow N_2 + 2OH^- + 2H_2O 
\tag{4}
\]
In this writing, just the nitrification section has been simulated.

**Modeling Equation**: The classical Euler–Euler two fluid model was employed to simulate the bubbly flow for every phase.

The equation of continuity for each phase is

\[
\frac{\partial (\varepsilon_k \rho_k)}{\partial t} + \nabla (\varepsilon_k \rho_k u_k) = S_k
\]

(5)

Where \( \varepsilon, \rho \) and \( u \) are gas hold-up, density, and velocity in each phase, respectively. \( S_k \) represents a source term of phase \( k \) in the domain.

**Momentum Equation Is Derived as Following**:\[
\frac{\partial (\alpha_k \rho_k u_k)}{\partial t} + \nabla (\alpha_k \rho_k u_k u_k) = -\alpha_k \nabla p + \alpha_k \rho_k g + \nabla \alpha_k t_k + F_{int}
\]

(6)

The right side of the above equation respectively shows pressure difference, gravity force, stress, and the ensemble averaged momentum exchange between the intra-phase forces. The pressure is shared between the phases [22, 23].

The drag and lift forces can be determined using equations (5) and (6), respectively:

\[
F_d = \frac{3}{4} C_d \frac{d_k}{d_b} \rho_1 \alpha_k \alpha_l |u_k - u_l|(u_k - u_l)
\]

\[ C_d = 0.622 \left( 1 / Eo + 0.235 \right) \]

(7)

(8)

Where, \( d_b \) is bubble diameter, \( CD \) is the drag coefficient and \( Eo \) is Eotvos number [22].

\[
F_l = -C_l \rho_1 \alpha_k \rho_l (u_k - u_l)
\]

\[ C_l = -0.06 \]

(9)

(10)

Where, \( CL \) is the lift coefficient.

The turbulent stresses can be evaluated using the following expression:

\[
\tau_k = -\mu_{eff} \left( \nabla u_k + (\nabla u_k)^T - \frac{2}{3} I (\nabla u_k) \right)
\]

(11)

Where, \( \mu_{eff} \) is the effective viscosity.

**Turbulence Equations**: The turbulent viscosity is governed by the \( k - e \) model [22] as following:

\[
\mu_t = \rho_t C_{t} \rho \frac{k^2}{e}
\]

(12)

The transport equation for the turbulent kinetic energy \( (k) \) and the evolution of the turbulent energy dissipation rate \( (e) \) are defined as following:

\[
\rho_t \frac{\partial k}{\partial t} - \nabla \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + \rho_t u_j \nabla k = \frac{1}{2} \mu_t (\nabla u_j + (\nabla u_j)^T)^2 - \rho_t e + S_k
\]

(13)

\[
\rho_t \frac{\partial e}{\partial t} - \nabla \left[ \left( \mu + \frac{\mu_t}{\sigma_e} \right) \nabla e \right] + \rho_t u_j \nabla e = \frac{1}{2} C_{e1} \frac{e}{k} \mu_t (\nabla u_j + (\nabla u_j)^T)^2 - \rho_t C_{e2} \frac{e^2}{k} + \frac{e}{k} S_k
\]

(14)

The model contains five parameters and those values were obtained from the literature as following [22, 24].

\[ C_{e1} = 0.09, C_{e2} = 1.44, C_s = 1.92, \sigma_k = 1.0, \sigma_e = 1.3 \]

Convection and diffusion have been studied using the following expression:

\[
\frac{\partial C_n}{\partial t} + \nabla (D \nabla C_n) = R - \alpha \nabla c \cdot NH_4
\]

(15)

Which \( C_n \) (n = 1-4) are the concentration of (NH₄⁺, NO₂⁻, NO₃⁻, O₂) respectively.

In this simulation, there are two reactions that happen continuously because of the enthalpy and entropy and diffusion coefficient for its material both reactions are sensitive to temperature so the heat effects are considerable.

The combination of mass balance for (NH₄⁺, NO₂⁻, NO₃⁻ and O₂) constitutes a set of four second-order differential equations with the following expression:

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 D_{rn} \frac{dC_n}{dr} \right) + r_i = 0
\]

Where \( r_n \) is the net reaction rate and \( D_{rn} \) the diffusion coefficient of each compound. By solving the equation, reaction rates were obtained as follows in Table 1.
Reactions details and heat settings have been introduced in Tables 2, 3.

The reactor consists of a tubular section of 0.085 m interior diameter and 0.8 m height with a conic bottom used as a settler. The fluidization zone between the air injection and the liquid level is 0.505 m high [25]. Half of the reactor has been selected for simulation and the processes were simulated at room temperature (25°C), except the simulation that concerns the temperature effects. For temperature effect simulation 15, 20, 25, 30°C were selected.

Feeding flow rate was 0.2, 0.6, 0.8 L/h which is water plus ammonia with the concentration of 250, 500, 750 mg/L. We assumed that 21% of air injection is oxygen and the rest is nitrogen and all of the oxygen is dissolved in the liquid. The bubbly flow regime was selected with the bubble size of $2 \times 10^{-3}$ m [26-27].
RESULTS AND DISCUSSION

In Figure 1, boundary setting (Figure 1-a), mesh element sizes (Figure 1-b), liquid and gas streamlines (Figure 1-c), liquid and gas volume fraction (Figure 1-d, f) and materials concentrations have been shown consecutively at the aeration of 2.26 L/h. It can be seen that the gas leaves the reactor but the liquid circulates in it.

Because of air injection from the center and bottom of reactor, these bubbles containing O₂ are new and fresh in lower zone concentration also the volume fraction of air is higher in this zone, so most of the reactions carried out here result in NO₃⁻ concentration becoming more than the other places also both reactions were carried out continuously thus when the first molecules of NO₂⁻ produced the other, the reaction was carried out quickly and NO₃⁻ starts being produced and because the most of oxygen and NO₂⁻ is in here, the second reaction carried out here is more than any other place so there is more NO₃⁻ concentration here.

Effect of Temperature: Figure 2 shows the temperature effect. By starting the first reaction, NH₄⁺ and O₂ decrease but the O₂ curve slope is more because it is consumed in two reactions.

About NO₃⁻, at first, the production rate is more than NO₂⁻ because the amount of NH₄⁺ that produces NO₂⁻ is more than NO₂⁻ that produces NO₃⁻ (at 25°C) until NH₄⁺ is finished, at this point, NO₂⁻ production rate turns negative because it is consumed in the second reaction. In addition, about NO₂⁻ the curve has two slopes, when NO₂⁻ is produced, the NO₂⁻ production slope is more but when NH₄⁺ is finished, with the slope of the NO₂⁻ production, NO₂⁻ producing slope decrease too. At high temperature the curve slope of NH₄⁺ and O₂ consumption are more, because the reactions are carried out quickly so the NO₂⁻ production rate increases but at lower temperatures at first the NO₂⁻ curve is near the zero because NO₂⁻ production is little and as soon as a little NO₂⁻ is produced, it is consumed too. About NO₃⁻, the curve has two slopes, at first where NO₂⁻ is produces, production rate of NO₃⁻ is high too, but as soon as the NO₂⁻ production finishes,
Fig. 2: Temperature effect. a) 15°C b) 20°C c) 25°C d) 30°C at feed flow rate of 0.8 L/h with 250 mg/L NH₄⁺

Fig. 3a: feed flow rate of 0.2 L/h with 250 mg/L NH₄⁺, b: at feed flow rate of 0.6 L/h with 250 mg/L NH₄⁺ at 25°C

the rate of NO₃⁻ production decreases too. Generally, NO₃⁻ production rate depends on NO₂⁻, meaning by increasing NO₂⁻ production, NO₃⁻ increase too and the opposite.

Effect of Feed Flow Rate: Figure 3, shows the effect of feed flow rate. Three different feed flow rates have been used 0.2, 0.6 and 0.8 L/h so that the last one is in Figure (2-c) at higher flow rate (0.6 L/h) the oxygen curve
Fig. 4a: Feed flow rate of 0.8 L/h with 500 mg/L NH4 at 25°C. b: at feed flow rate of 0.8 L/h with 750 mg/L NH4.

Fig. 5a: Temperature effect. Feeding flow rate of 0.8 L/h and 250 mg/L NH4.

Fig. 5b: Feeding flow rate effect. 250 mg/L NH4 concentration at 25°C.

Fig. 5c: NH4 concentration effect. Feeding flow rate of 0.8 L/h at 25°C.
We can see that with the increase of $NH_4^+$, the rate of consuming and producing of the material is smoother. In lower concentrations of $NH_4^+$ there are two cross points between NO$_2$ and NO$_3$; one of which is at increasing of both of them and the other is when NO$_2$ is consumed and NO$_3$ is produced because when $NH_4^+$ increases and O$_2$ is stable, O$_2$ isn’t enough and in addition reactions are competing so NO$_2$ is consumed but it has been substituted and NO$_3$ consumption isn’t clear but when $NH_4^+$ is less, O$_2$ is enough to consume all the NO$_2$, exactly that’s why when $NH_4^+$ decreases, the difference between the slopes in every material is more clear, in addition the first cross point has done it sooner, as much as $NH_4^+$ increase, the cross point happens later.

Figure 5, shows the comparison between our simulation and the simulation in the reference for the experimental data. In all of them the vertical axis is NO2/NO4 ratio and the other is dissolved oxygen concentration. Figure 5.a is about temperature effect. Figure 5.b feeding flow rate effect and Figure 5.c is $NH_4^+$ concentration effect. The results show desirable agreement between our simulation and the reference simulation but there is a little difference about the slope of charts its maybe because of some assumptions for example in the reference article liquid is imported from the top of the reactor and gas from the bottom but in our simulation both liquid and gas are imported from the bottom and this assumption effects the reaction time because it decreases the time that oxygen is taken to $NH_4^+$. When oxygen comes from the top, time increases so the oxygen consumption for a special ratio increases so the chart slope changes but the amount of oxygen for all of the $NH_4^+$ doesn’t change.

In Figure 6, the experimental results of O2/N-$NH_4^+$ influences on the N-NO2 / N-$NH_4^+$ and in Figure 7 the effect of DO concentration on N- compounds distribution has been shown experimentally as well as the simulation, these figures are two samples, all the other figures (from reference [25] simulation ) have been compared with the experimental once (in the original article) and have shown suitable agreement is indicated between them so we have compared our simulation results with the simulation of the reference article [25].

CONCLUSIONS

The effects of temperature, ammonium concentration and feed flow rate on nitrifying treatment of wastewater in an airlift reactor have been simulated in this article.
The simulation results showed that at higher temperatures, reactions are carried out quicker so the curve slope of NH₄⁺ and O₂ consumption is higher. At higher feed flow rates at first the accumulation of NO₂ increases, if there is enough O₂, the second reaction for producing NO₃ will speed up until all amount of NO₂ is consumed and we can see that with the increase of NH₄⁺, the rate of consuming and producing of the material is smoother. All the simulation results were compared with experimental data that have shown a suitable agreement.

Nomenclature

- $C_d$: Drag force coefficient
- $C_l$: Lift force coefficient
- $C_o$: Constant in k-ε model
- $C_{ir}$: Model parameter in turbulent dissipation energy equation
- $C_{ire}$: model parameter in turbulent dissipation energy equation
- $d$: [m] bubble diameter
- $F$: [N/m²] Interaction forces
- $E_o$: Eotvos number

Greek symbols

- $\alpha$: Prandtl number for turbulent energy dissipation rate
- $\alpha_k$: Prandtl number for turbulent kinetic energy
- $\tau$: [N/m²] Stress tensor of phase k
- $\epsilon$: [m²/s] Turbulent dissipation rate per unit of mass
- $\omega$: Volume fraction of phase k
- $\mu$: [Pa-s] Viscosity of phase k
- $\rho$: [kg/m³] Density of phase k
- $N$: [m/s] Kinematic viscosity

Subscript

- k: phase, k = G: gas phase, k=L: liquid phase

REFERENCES


