International Journal of Academic and Applied Research (IJAAR)
ISSN: 2643-9603
Vol. 4, Issue 7, July – 2020, Pages: 82-87

NanoCalc Simulation and Modellings of Silver Nanoparticles for direct Antimicrobial Coatings

Olabimtan Olabode H.[*1], Ochigbo Victor[2], Ashade Noah O.[3]

[1]Department of Industrial and Environmental Pollution, National Research Institute for Chemical Technology Zaria, Kaduna State, Nigeria.
[2]Department of Scientific and Industrial Research, National Research Institute for Chemical Technology Zaria Kaduna State, Nigeria.
[3]Research and Development, Outstation Coordination Department, National Research Institute for Chemical Technology Zaria Kaduna State, Nigeria.

Corresponding author email*: *Olabode4angel@gmail.com*

Abstract: *Bacterial infections, especially by antimicrobial resistant (AMR) bacteria, are increasing problems worldwide. AMR is especially a problem with health care-associated infections due to bacteria in hospital environments being easily transferred from patient to patient and from patient to environment, and thus, solutions to prevent bacterial transmission are needed. Hand washing is an effective tool for preventing bacterial infections, but other approaches such as nanoparticle-coated surfaces are also needed. In this study, android based nanoparticles application was direct simulated and modelled to the advantage of silver nanoparticle antimicrobial coated surfaces. The nanoparticles with possible precursors on the basis of their diameter (nm), initial concentration (uM) and volume (ml) between 1 to 10 in each cases modelled respectively against the average and total surface areas in* nm^2*, average and total volume in* nm^3*, average mass in gram, dosage in ug/ml and final concentrations in uM. The graphical models between the average Ag NP diameter with the average surface area [* $y=0.8527x^{0.25}$ *[x* $\times 10^{15}$*] (* $R^2=1$*)]; average volume [*$y=1.2425x^{0.333}$ *(*$R^2=1$*)], mass [*$y=5.6682x^{0.3333}$ *[*$x\times10^{-18}$*] (*$R^2=1$*)]; total surface area [y=* $0.8527x^{0.25}$*[*$x\times10^{-18}$*](*$R^2=1$*)], total volume [*$y=0.7947x^{0.2}$ *(*$R^2=1$*)], dosage [*$y=0.7414x^{0.25}$ *(*$R^2=1$*)] and final concentration [*$y=0.3632x^{0.2603}$ *(*$R^2=0.9398$*)]. Between the initial concentration and average surface area [*$y=0.5637x^{0.5002}$ *(*$R^2=1$*)], average volume[*$y=1.2425x^{0.333}$ *(*$R^2=1$*)],mass[*$y=5.6682x^{0.3333}$ *(*$R^2=1$*)], total surface area[*$y=0.8527x^{0.25}$*[*$x\times10^{15}$*] (*$R^2=1$*)], total volume[*$y=0.7947x^{0.2}$*[*$x\times10^{14}$*] (*$R^2=1$*)], dosage [*$y=0.7414x^{0.25}$ *(*$R^2=1$*)] and final concentration [*$y=0.3632x^{0.2603}$ *(*$R^2=0.9398$*)] and with initial aqueous volume against the average surface area [*$y=0.5637x^{0.5002}$ *(*$R^2=1$*)], average volume [*$y=1.2425x^{0.333}$ *(*$R^2=1$*)], mass [*$y=5.6682x^{0.3333}$*[*$x\times10^{-18}$*] (*$R^2=1$*)], total surface area[*$y=0.8527x^{0.25}$*[*$x\times10^{15}$*] (*$R^2=1$*)], total volume[*$y=0.7947x^{0.2}$ *[*$x\times10^{14}$*](*$R^2=1$*)], dosage[*$y=0.7414x^{0.25}$ *(*$R^2=1$*)] and final concentration [*$y=0.3632x^{0.2603}$ *(*$R^2=0.9398$*)].Preparation of silver coated antimicrobial coatings on solid surfaces and many other application can be systematically achieved with this simple and user friendly applications. However, further validation and claim are necessary for wide applications and acceptance.*

Keywords: NanoCalc, modelling, simulation, silver nanoparticles and antimicrobial coatings.

1.0 INTRODUCTION

Bacterial infections have significant global implications with antimicrobial-resistant infections [1]. Antibacterial activity-resistant is a known global challenge as it has been estimated that more of 10 million deaths globally will be linked with antimicrobial-resistant bacteria by the year 2050[2]. A growing class of aged are being treated in the hospitals and geriatric institutions, and therefore with a likelihood of developing health care related complications. In health care facilities, pathogenic microbes are automatically shared through substrates like door knobs, tables, water-tap handles, toilet seats, bed linens, bed edges, trolleys, and transmission to others. The transmission may result into nosocomial pathogens which induce prolonged inpatient hospitalization, more severe infections and death, especially with the infection of antimicrobial-resistant bacteria like Escherichia coli and staphylococcus aureus. The most prevalent pathogens related with health care-associated infections, particularly fluoroquinolone-resistant E, were reported to be S.aureuses E Coli-strains [3]. Proper hand hygiene with ethanol-based solution are the effective way of preventing bacterial infection, against the recent investigation that the death rate from health care-associated infections was increased, due to multi-resistant bacteria [1]. Efficient tools against infections and antimicrobial-resistant bacteria are still required despite the improved hand hygiene. The promising innovation for avoiding bacterial infections and bacterial transmission in hospital environments is antimicrobial surfaces. Nanostructures as ultrafine materials are generally interpreted as particles of diameters within 1 and 100 nanometers (nm) [4]. The concept is applied for larger particles between 500 and100 nm tubes and fibers as metal particles smaller to 1 nm are typically called fragments or clusters of atoms at the lowest level instead. Nanoparticles are generally distinguished from microscopic particles (1-1000 μm), as fine particles ranging from 100 to 2500 nm, and coarse particles between 2500 and 10,000 nanometer with smaller sizes generating different physicochemical

properties like colloidal and optical or electrical properties[5]. Typically, because they are more prone to tyndall movement, they do not precipitate like colloidal particles, which are generally acknowledged to scale from 1 to 1000 nm [4]. Since nanoparticles are much smaller, the visible light wavelengths (400- 700 nm) cannot be identified using basic optical microscopes but with high resolution electronic microscope [4]. Dispersions of nanoparticles through transparent materials may be invisible for the same purpose, while suspensions of larger particles typically spread all the visible incidents light [4]. Nanoparticles often easily pass through modern ceramic filters that requires unique nanofiltration systems [4]. The specific characteristics of nanomaterial usually varies significantly with the larger particles. As the average length with the atom rest within 0.15 to 0.6 nanometer, a substantial percentage of the particles are from the surface with some diameters [6]. The nanoproperties of the surface layer can then prevail over those of the bulk material, as the effect is especially strong for nanoparticles dispersed in a medium of different composition, because the interactions between the two materials at their interface have become important [4].One key aspect with nanotechnology is the development of nanoparticles with unique properties with smaller dimension of nanoparticles which often results in a lower composition relative with the particles in the bulk of the materials, without the support of displacements under the modified microscopy (electron) [4]. Nanoparticles, furthermore, demonstrate different modification pathways which, alongside their specific structural features, results with mechanical characteristics that are different from the normal material. Different metallic nanoparticles, such as Ag, TiO_2, Cu_2O and ZnO, are considered to be antimicrobial as they interfere with the bacterial bio formation by hindering the proton cell envelope pumps with DNA replication. Meanwhile, diverse antimicrobial requirements, particularly biomedical nanoparticles for textiles, metal nanoparticles, particularly silver nanoparticles, have shown impressive potentials [7]. Technically, Silver nanoparticles induce DNA damage, deactivate enzymes, trigger cell termination by enhancing membrane fluidity, and by changing the geometry of membranes it may as well be adopted for antimicrobial treatment[9].The benefits of utilizing silver nanoparticles is centered on their composition as nanoparticles of 0.2–100 nm in size with high surface to volume proportion with the advantage of effective reactivity against the microbes .Explicitly silver nanoparticles are between one and one hundred nanometer in dimension as some are the composition of higher proportions with oxide of silver owing to its high coefficient of silver atoms to mass. The potentials and activities achieved via their special physicochemical characteristics, silver nanoparticles are increasingly been applied in various areas like health care, medicinal, food, industrial and consumer purposes. Similarly, properties like high electrical conductivity, mechanical, thermal and biological properties are being exploited as antibacterial parameters, active chemical, health-related products, consumer products, medical equipment coatings, optical devices and cosmetic products, pharmaceutical, diagnostic devices, orthopedics and delivery of drug as an anti-cancer agent [11]. They have currently been utilized extensively in several biomedical devices, textiles, keyboards and wound dressings. In order to satisfy the silver nanoparticles requirement, different techniques for the synthesis have been identified. Conventional chemical and physical approaches seem very toxic and costly while biologically formulated nanoparticles demonstrate high stability, yield and solubility [12]. Biological methods emerge to be simple, rapid, non-toxic, dependable, and green approaches among several synthetic methods for silver nanoparticles that can generate excellently-defined surface morphology under optimized synthetic conditions. During military campaigns silver receptacles were engaged for water transportation, and silver salts were also used to store water and food [13]. Historically, the adoption of silver antimicrobial and preserving agent was from 4000 BC as the early explorers traveling long distances around the North American continent used a similar method by dropping a silver coin into their water or milk [14]. Metal salts such as mercury, silver, zinc and copper were adopted by the Egyptians, Greeks and the Romans in cleaning of wounds with silver strings [15]. As well, down the 20th century, the adoption of silver based salts to clean wounds and to promote healing remained as the treatment of bruises with silver sutures was more effective in preventing infections[16],[17]. Silver nitrate compounds have also been used to fight infections just like the eye drops against eye infections [18]. The first application of silver colloids for wound antisepsis was documented in the late 19th century as silver nitrate was a general treatment before the discovery and development of antibiotics in the 20th century [13]. Silver can be applied in various ways, either as powder, as a compound or as a free dissolved ion. The prehistoric silver consumers had no idea the form of silver that worked best while they only noted the beneficial benefits of silver salts. It was as well discovered that silver performed best with some moisture as established recently that silver ion (Ag^+) has antimicrobial activity [19]. Since the advent of penicillin antibiotics in the 1940s, silver use diminished. Silver nitrate solutions were, however, reincorporated against injuries in the 1960s, and was advanced with the emergence of silver sulfadiazine [20]. This compound significantly reduced the degree of infection but however later discovered with slow healing effects, therefore was not recommended any more. The invention of silver nanoparticles improves the silver use heavily with the substantive claims of strong antimicrobial activity [21]. It is still questionable how exactly silver nanoparticles exert anti-microbial activity. However, it was proposed that small particles may exhibit nano-toxicity due to the small size combined with varying properties and in vitro experiments that shown that high concentrations of

International Journal of Academic and Applied Research (IJAAR)
ISSN: 2643-9603
Vol. 4, Issue 7, July – 2020, Pages: 82-87

silver nanoparticles have adverse effects on cells [22]. Meanwhile, the safety of Ag NPs are yet to be ascertained on patient despite its valuable chemical nature as used in a range of applications. Therefore, the laboratory development of Ag NPs were directly simulated and modelled for the comprehensive definitions of it characteristic feature, such as size, shape, size distribution, surface area, shape and solubility for biocompatibility and antimicrobial activities. [23]

2.0 METHODOLOGIES

Nanoparticle Calculator -NanoCalc -as a project aimed at creating an Android framework for the measurement of nanoparticles' physical parameters. By integrating the diameter, concentration and solution volume of the NPs, NanoCalc computes the mass, surface area, volume of the single nanoparticles, total number of nanoparticles, total surface area exposed and total volume taken up by the nanoparticles

Table 1. NanoCalc Simulations of Ag nanoparticles

Ag NP diameter (nm)	Ag NP initial Conc. (uM)	Ag NP initial solution Volume (ml)	Single Ag NP S. Area (nm^2)	Single Ag NP volume (ml)	Single Ag NP mass(g) ($X10^{-18}$)	Total Ag NP ($X10^{14}$)	Total Ag NP mass(g) ($X10^{-1}$)	Total Ag NP S. Area(nm^2) ($X10^{15}$)	Total Ag NP volume (ml) ($X10^{14}$)	Ag NP Dosage (ug/ml)	Final Ag NP Conc.(uM)
1	1	1	3.14	0.52	0.00549	602.00	0	1.89	3.15	3.31	30.70
2	2	2	12.60	4.19	0.04390	24.10	0.0011	30.30	101.00	52.90	4910.00
3	3	3	28.30	14.10	0.14800	54.20	0.0080	153.00	766.00	268.00	2480.00
4	4	4	50.30	33.50	0.35200	96.40	0.0339	485.00	3230.00	847.00	7850.00
5	5	5	78.50	65.40	0.68700	151.00	0.1030	1180.00	9850.00	2070.00	19200.00
6	6	6	113.00	113.00	1.19000	217.00	0.2570	2450.00	24500.00	4290.00	39700.00
7	7	7	154.00	180.00	1.88000	295.00	0.5560	4540.00	53000.00	7940.00	73600.00
8	8	8	201.00	268.00	2.81000	385.00	1.0800	7750.00	103000.00	13500.00	126000.00
9	9	9	254.00	382.00	4.00000	488.00	1.9500	12400.00	186000.00	21700.00	201000.00
10	10	10	314.00	524.00	5.49000	602.00	3.3100	18900.00	315000.00	33100.00	307000.00

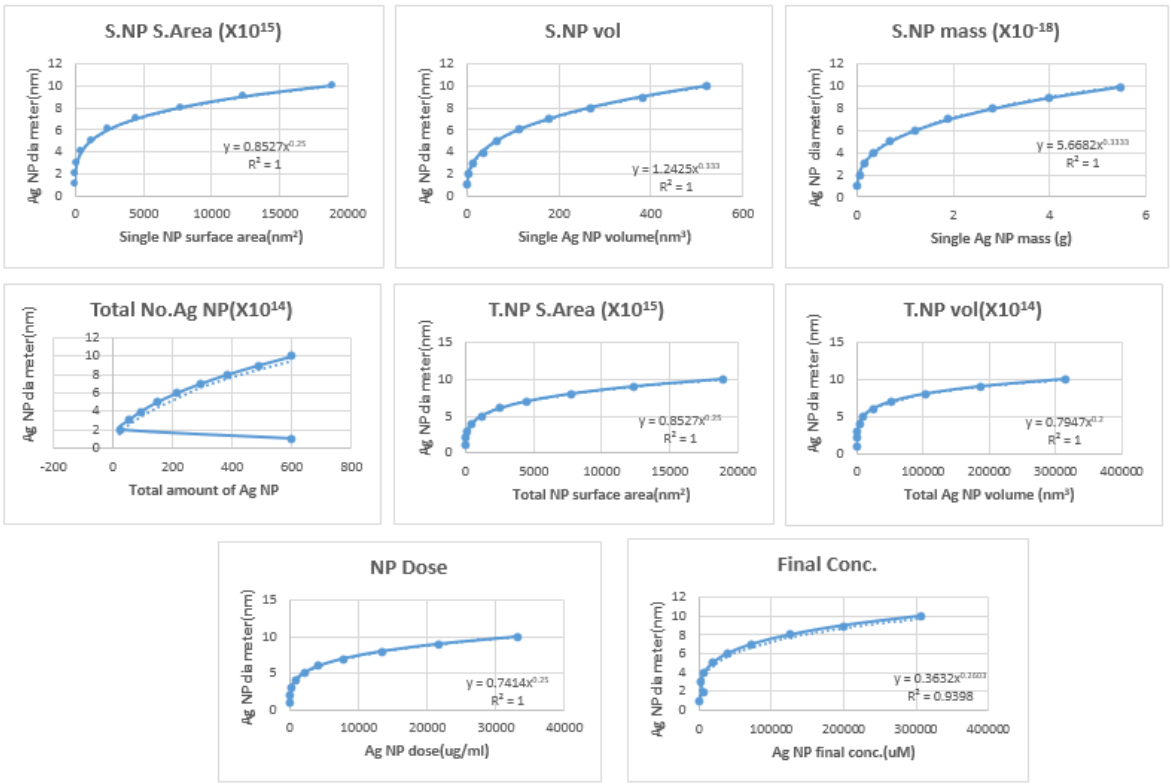

Figure 1. Graphical Modellings of an average Ag nanoparticle diameter (nm) against its surface area (nm^2) [$x\times10^{15}$], volume (nm^3), mass (g) [$x\times10^{-18}$], amount (number), total surface areas (nm^2) [$x\times10^{14}$], total volume (nm^3), dosage (ug/ml) and final concentration (uM).

International Journal of Academic and Applied Research (IJAAR)
ISSN: 2643-9603
Vol. 4, Issue 7, July – 2020, Pages: 82-87

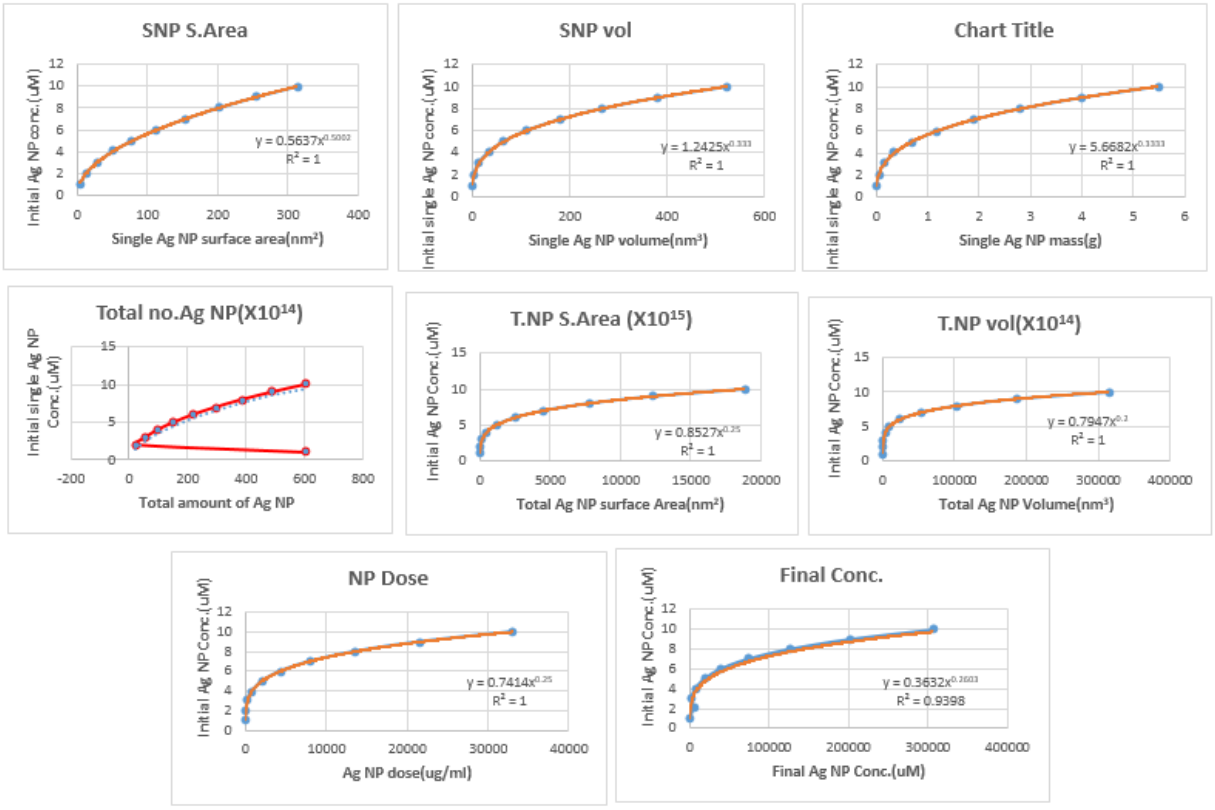

Figure 2. Graphical Modellings of initial Ag nanoparticle concentration (uM) against its surface area (nm^2), volume (nm3), mass (g), Amount (number), total surface areas (nm^2) [$x \times 10^{15}$], total volume (nm^3) [$x \times 10^{14}$], dosage (ug/ml) and final concentration (uM).

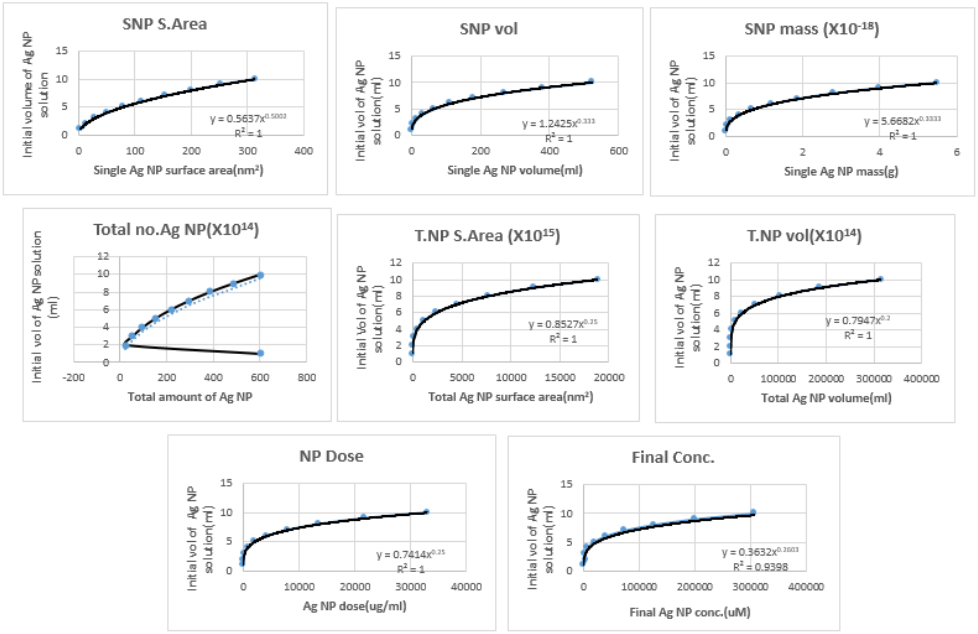

Figure 3.Graphical Modellings of initial Ag nanoparticle solution volume (ml) against its surface area (nm^2), volume (nm^3), mass (g) [$x \times 10^{-18}$], Amount (number), total surface areas (nm^2) [$x \times 10^{15}$], total volume (nm^3) [$x \times 10^{14}$], dosage (ug/ml) and final concentration (uM).

International Journal of Academic and Applied Research (IJAAR)
ISSN: 2643-9603
Vol. 4, Issue 7, July – 2020, Pages: 82-87

Table 2. Power modellings of Ag nanoparticles

	Single Ag NP Surface area(nm^2)		Single Ag NP volume(nm^3)		Single Ag NP mass (g)		Total Ag NP Surface area(nm^2)		Total Ag NP Volume(nm^3)		Ag NP Dose (ug/ml)		Final Ag NP Conc.(uM)	
	Model Equation	R^2	Model Equation	R^2	Model Equation	R^2	Model Equation	R^2	Model Equation	R^2	Model Equation	R^2	Model Equation	R^2
Ag NP diameter(nm)	$Y=0.8527x^{0.25}$	1	$Y=1.2425x^{0.333}$	1	$Y=5.6682x^{0.3333}$	1	$Y=0.8527x^{0.25}$	1	$Y=0.7947x^{0.2}$	1	$Y=0.7414x^{0.25}$	1	$Y=0.3632x^{0.2603}$	0.9398
Ag NP initial Conc.(uM)	$Y=0.8527x^{0.25}$	1	$Y=1.2425x^{0.333}$	1	$Y=5.6682x^{0.3333}$	1	$Y=0.8527x^{0.25}$	1	$Y=0.7947x^{0.2}$	1	$Y=0.7414x^{0.25}$	1	$Y=0.3632x^{0.2603}$	0.9398
Ag NP Initial aqueous Volume(ml)	$Y=0.8527x^{0.25}$	1	$Y=1.2425x^{0.333}$	1	$Y=5.6682x^{0.3333}$	1	$Y=0.8527x^{0.25}$	1	$Y=0.7947x^{0.2}$	1	$Y=0.7414x^{0.25}$	1	$Y=0.3632x^{0.2603}$	0.9398

The simulations eventually modelled the synthesis of silver nanoparticles with reference to their surface areas, volumes, masses, dosages and final concentrations. As the production of silver nanoparticles are typically achieved with any chemically stabled precursors which can be directly simulated with the input factors of their diameters in nanometer and initial concentration and volume in micromolar and milliliters respectively. As disclosed on table 1, the simulator (NanoCalc) generated modelled runs in terms of single silver nanoparticles surface area, volume, mass and total surface area, volume, dose and final concentration. They were adopted in the plotting of the nano silver diameters, initial concentration and initial aqueous volume against them accordingly. (Figure 1, 2 and 3).The modeled relationships that were established excluding the total number of nanoparticle justifies the achieved correlational coefficients in each cases (Table 2).

3.0 CONCLUSION

The project evaluated the validity of android based nanoparticles applications on the development of silver nanoparticles over three dimensional surfaces that could prevent bacterial transmission especially in hospital environments. It has been established that with the direct application of NanoCalc application, silver based nanoparticles can easily be produce with the economy of reactants (silver compound precursors and the stabilizing agents) with input and output predictions for antibacterial surface coatings. The modellings clearly established the relationships and the effects between the necessary variables as identified by the application.

4.0 RECOMMENDATIONS

Antimicrobial properties of silver nanoparticle applying this models should be explored against the notorious *E- coli* and *Staphylococcus aureus.*

5.0 REFERENCE

1. Gunell M et al (2017). Antimicrobial characterization of silver nanoparticle-coated surfaces by “touch test” method. Nanotechnol Sci Appl.;10:137-145 https://doi.org/10.2147/NSA.S139505
2. Ferri, M.et al (2015). Antimicrobial resistance: A global emerging threat to public health systems. Critical Reviews in Food Science and Nutrition, 57(13), 2857 2876. doi:10.1080/10408398.2015.1077192
3. Lee, D. S.et al (2018). Community-Acquired Urinary Tract Infection by Escherichia coli in the Era of Antibiotic Resistance. BioMed Research International, 2018, 1–14. doi:10.1155/2018/7656752
4. Nanoparticle. En.wikipedia.org. (2020). https://en.wikipedia.org/wiki/Nanoparticle.
5. Nanoparticles | Peer Reviewed Journals. Longdom.org. (2020). https://www.longdom.org/peer-reviewed-journals/nanoparticles-27944.html.
6. Nanoparticle. Newikis.com. (2020). https://newikis.com/en/Nanoparticle.
7. Xu L et al (2020). Silver nanoparticles: Synthesis, medical applications and biosafety. Theranostics 10(20):8996-9031. doi:10.7150/thno.45413. http://www.thno.org/v10p8996.htm
8. N. Thajuddin and Silvy Mathew (2020).Phytonanotechnology https://www.sciencedirect.com/book/9780128223482/phytonanotechnology.
9. Vardanyan, Z.et al (2015). Effects of various heavy metal nanoparticles on Enterococcus hirae and Escherichia coli growth and proton-coupled membrane transport. Journal of Journal of Nanobiotechnology, 13(1). doi:10.1186/s12951-015-0131-3
10. Fatima, F.et al (2016). Extracellular mycosynthesis of silver nanoparticles and their microbicidal activity. Journal of Global Antimicrobial Resistance, 7, 88–92. doi:10.1016/j.jgar.2016.07.013
11. Zhang, X. F.et al (2016). Silver Nanoparticles: Synthesis, Characterization, Properties, Applications, and Therapeutic Approaches. International journal of molecular

sciences, 17(9), 1534. https://doi.org/10.3390/ijms17091534

12. Varghese, B et al (2020). Biochemical synthesis of copper nanoparticles using Zingiber officinalis and Curcuma longa: Characterization and antibacterial activity study. Materials Today: Proceedings. doi:10.1016/j.matpr.2020.01.476
13. Knetsch, M. L. W., & Koole, L. H. (2011). New Strategies in the Development of Antimicrobial Coatings: The Example of Increasing Usage of Silver and Silver Nanoparticles. Polymers, 3(1), 340 366. doi:10.3390/polym3010340
14. Spear, M. (2010). Silver: An Age-Old Treatment Modality in Modern Times. Plastic Surgical Nursing, 30(2), 90–93. doi:10.1097/psn.0b013e3181deea2e
15. Knetsch, M.L.W.and Koole, L.H (2011). New Strategies in the Development of Antimicrobial Coatings: The Example of Increasing Usage of Silver and Silver Nanoparticles. Polymers, 3, 340-366.
16. White, R. J. (2001). An historical overview of the use of silver in wound management. British Journal of Community Nursing, 6(Sup1), 3–8. doi:10.12968/bjcn.2001.6.sup1.12619
17. Paladini, F., & Pollini, M. (2019). Antimicrobial Silver Nanoparticles for Wound Healing Application: Progress and Future Trends. Materials (Basel, Switzerland), 12(16), 2540. https://doi.org/10.3390/ma12162540
18. Ray Sahelian, M.D (2016).Colloidal Silver benefits and risks.https://www.raysahelian.com/colloidalsilver.html.
19. Microbewiki (2020). Silver as an Antimicrobial Agent http://microbewiki.kenyon.edu/index.php/Silver_as_an_Antimicrobial_Agent.
20. Taliyah, B. S.et al (2007). Effect of silver on burn wound infection control and healing: Review of the literature. Burns, 33(2), 139–148. doi:10.1016/j.burns.2006.06.010
21. Losasso, C.et al (2014). Antibacterial activity of silver nanoparticles: Sensitivity of different Salmonella serovars. Frontiers in Microbiology, 5. doi:10.3389/fmicb.2014.00227
22. Pellissari, et al (2020). In Vitro Toxic Effect of Biomaterials Coated with Silver Tungstate or Silver Molybdate Microcrystals. Journal of Nanomaterials, 2020, 1–9. doi:10.1155/2020/2971827
23. Android - Nanoparticle Calculator. (2020). https://steprimo.com/android/us/app/appinventor.ai_giuseppevec.Nano_Calc/Nanoparticle-Calculator/.