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(Volume No. 12, Issue No. 1 January - April 2024)

Sr No	Article/Autors	Pg No
51. 100		1 g 10
01	<ul> <li>Modeling and Analysis of Machining Parameters on Surface Roughness and Cutting Force In Finish Dry Hard Turning (FDHT) of AISI D2 Tool Steel By RSM Approach</li> <li><i>Vaibhav Chandra<sup>1,2‡</sup>, Umesh Khandey<sup>2</sup>, Sudarshan Ghosh<sup>3</sup>, P.V. Rao<sup>4</sup></i></li> </ul>	01-13
02	Second Law Efficiency and Exergy Destruction Analysis of Vapour Compression Refrigeration System -Ashfaque Ahmad, Faizan Ali, Himanshu Bhardwaj, Md Asfar, Md Jamshed Khan, Meraj Ahmad and Sadia Aman	14-24
03	Study of Fluoride level in the Ground Water of Western Uttar Pradesh (India) - Weqar Ahmad Siddiqui, Mohd Waseem#	25-30
04	Urban Rain Water Harvesting – Need and Comprehensive Approaches - Sirajuddin Ahmed <sup>1</sup> RupinderNarang <sup>1*</sup> and Rajkumar Joshi <sup>2</sup>	31-38
05	Microwave Assisted Rapid Synthesis of Some Schiff Bases and Their Antimicrobial Activity - Mrunal M. Mahajan, Pravin B. Raghuwanshi	39-48

# Modeling and Analysis of Machining Parameters on Surface Roughness and Cutting Force In Finish Dry Hard Turning (FDHT) of AISI D2 Tool Steel By RSM Approach

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# ABSTRACT

AISI D2 tool steel material is considered as difficult material to be machined. It exhibits various properties such as high wear resistance, high hardness, high strength and rapid strain hardening etc. In the present work, Response Surface Methodology (RSM) has been used to investigate the effect of four major influencing machining parameters on surface roughness and cutting forces. The parameters namely cutting speed, feed rate, depth of cut and rake angle have been considered for dry machining of AISI D2 tool steel. The secondorder polynomial model has been constructed for cutting force and surface roughness. The adequacy of model has been checked though analysis of variance (ANOVA) and found to be best fitted for prediction of surface roughness and cutting forces. The Coefficient of Determination ( $R^2$ ) for surface roughness and cutting force has been found to be 90.19% and 98.33% respectively.

Keywords-AISID2 Steel; FDHT; RSM; Cutting Force; Surface Rouhness.

## **1. INTRODUCTION**

Now a days coated cutting inserts are widely accepted by the metal cutting industries to machine the materials which are difficult to cut. They used to decrease the tool wear due to their significance properties, like high temperature oxidation resistance, great tribological properties, high wear strength, etc. To perform the hard turning correct combination of cutting tool material, feed rate, depth of cut, cutting speed, insert geometry is required, so that better results can be achieved in single cut of turning rather than in multiple cut of finishing operations. Hard turning is performed on those engineering materials whose hardness is more than 45 HRC level.

It is the most appropriate alternative of grinding operation or any other conventional surface finishing operation in terms of surface quality[1]. Therefore it serves as a grinding replacement process. The typical material which is hard turned are steel alloys, bearing steels, die steels, case hardened steels, etc. While performing the hard machining the various factors are need to be consider in terms of machine for ideal machining. These factors are machine rigidity, work holding rigidity, good vibration damping characteristics, rigid tool location, rigid cutting tools and advanced insert materials. Hard turning not only eliminate the requirement of grinding but also increase the rate of production by reducing the cycle time of finishing operation. It also reduces the cost of turning operation as well as setup time of machining. The large varieties of tool steel materials are classified by their applications, by their composition or by specific characteristic properties and others by the manner of heat treatment. The American Iron and Steel Institute (AISI) has published and classified the Tool steels into the various categories with identifying letter or symbols such as Water-Hardening tool steels (W), Shock-Resisting tool steels (S), High-Carbon, High Chromium (D) or AISI D2, Hot work Tool steels (H), Mould Tool Steels (P), etc. AISI D2 have a great application in the field of tooling industries, such as in making forging dies, dies of pressure die casting, and cutting dies apart for these they are also frequently used in the manufacturing of Jigs and fixtures, reamers, broaches, knives, Gauges, measuring tools, guide rails, bushes, sleeves, knurling tools etc. The main composition of AISI D2 is given in table 1. Similarly the mechanical and thermal properties of AISI D2 are given in table 2. Now a days lots of options are available for the metal cutting industries to choose the cutting inserts. But selection of appropriate cutting insert is great a challenge. There are various factors on which selection is depend such as work piece hardness, cutting temperature, tool life, process parameters, etc.

Elements	Weight %
Carbon	1.5
Silicon	0.3
Manganese	0.3
Molybdenum	1
Chromium	12
Nickel	0.3
Vanadium	0.8
Cobalt	1
Iron	Balance

Table 1 Chemical composition of AISI D2 steel work piece in percentage by weight.[2]

The EDAX testing has been done on our selected work piece which confirm the chemical composition as per literature as shown in figure 1.



Fig 1: Result of EDAX analysis of AISI D2 material

Thermal properties					
Thermal conductivity (W/m K)	21				
Specific heat capacity (J/kg K)	485				
Mechanical properties					
Young's modulus (GPa)	180				
Poisson's ratio	0.3				
Density (kg/m3)	7,750				
Hardness (HRC)	62±1				
Elongation (%)	=16				

Steel alloy are generally very hard for most the applications used, ranging between 45 to 65HRC. Such material comes up with lots of machining difficulties such as mechanical shock, generation of high temperature at the primary shear zone, high tool wear rate, dimensional distortion, precision requirement, etc. To overcome such issues inserts manufactures have done drastically changes in the inserts to perform the hard turning. Now a days PVD, CVD coated carbide, cermet, ceramic, cubic boron nitride (cBN), and polycrystalline diamond (PCD) inserts all play a key role. These advanced material inserts have special geometries and hard coatings of different materials withstand mechanical shock and heat while resisting abrasive wear, etc. These advanced cutting tools are able to achieve good surface quality and economic efficiency comparable to that of grinding operation. And also the possibility of excellent tool life, optimal process reliability. The current work investigate the effects of finish dry hard turning(FDHT) on cutting forces( $F_y$ ) and surface roughness ( $R_a$ ) with using of TiAlN coated carbide inserts of different geometry.

#### **2. LITERATURE REVIEW**

Now a days it is necessary to optimize the input parameters during cutting, such as feed rate, cutting speed and depth of cut. Optimization is an important tool extensively used in machining process in order to get the suitable range of parameters so that desired product quality can be achieved. Sahoo, et al.[4] done the comparative study on volume of chips, tool life, surface roughness, flank wear. To machined the AISI D2 material they selected multilayered TiN coated and uncoated carbide cutting inserts under dry condition. They observed that tool life is increases 30 times with multilayer TiN coated carbide insert and also lower surface roughness value. Sharma et al[5]. performed the study on AISI D2 using vegetable oil by using Tungsten carbide insert (CNMG12408). They compared the results with dry machining and near dry machining. According to the results near dry machining shows good results in terms of cutting temperature at work tool interface and roughness value. Dipti kanta das et al.[6] have perfomed dry turning on EN 24 steel. The model for predicting the surface roughness has been develpoed. They have identified feed rate as a most dominant parameter for surface roughness and concluded the adequecy of surface roughness model by correlation coefficient ( $R^2 = 0.993$ ). Sahoo and Sahoo[7] have developed mathematical modeling in hard turning of AISI 4340 steel using multilayer coated carbide insert. They have used RSM and Grey-based Taguchi approach for the optimization and mathematical modeling for the output characterstics. They have been found that the economical feasibility of their study and developed model fitted well for prediction and optimization. The dry turning of AISI 1040 mild steel has been performed by Noordin et al.[8]. They have studied the performance of coated carbide tools using response surface methodology and foud well for the judgment of performance of tool. Anderson Paulo, et al[9] implement the optimization theory based on the multi objective hybrid approach combining response surface methodology (RSM) with Principal Component Analysis (PCA) using AISI 52100 hardened steel. To turned the material they uses wiper mixed ceramic tools. Suresh et al.[10] investigated experimentally and optimized the machining conditions in turning of mild steel work piece using TiN-coated tungsten carbide. They adopted the Genetic Algorithms (GA) and RSM methodology to develop the prediction model of surface roughness.

## **3. EXPERIMENTAL SETUP**

### 3.1 Workpiece Material.

In the present study rod of AISI D2 having the size of diameter 95 mm and length of 300mm were used. As per the method of heat treatment the specimen is inserted into a salt bath furnace at 1000–1040 °C,

Journal of Dynamics of Fluids (Volume- 12, Issue - 1 January-April 2024 )

then quenched in oil, and finally tempered at low temperature ( $220^{\circ}$ C) for around 45 minutes to achieve the required hardness value of 55±1 HRC.

## 3.2 Machine Tool

The experimental investigation was made up of the CNC T-6 (Leadwell, Taiwan) lathe machine of 15 HP spindle power with maximum speed of 4500 rpm. It is installed at Central Workshop of Mechanical Engineering Department, IIT, Delhi, India

## 3.3 Cutting Tool

In the current work 5 levels were selected of rake angle. For CNMG inserts -6 degree default rake angle tool holder were used. And for VNMG insert -10 degree rake angle tool holder was used. The complete details of cutting inserts and effective rake angles are given in table 3.

ISO Specification	Effective rake
	angle
VNMG 160408 - SM 1105	-10
CNMG 120408 – MM 1115	-6
CNMG 120408 – MP KC 5025	0
CNMG 120408 – MS KC 5510	7
CNMG 120408 – FF KC 5010	14

## Table 3 Details of cutting inserts

## 3.4 Design of Experiments.

In this study cutting speed, feed rate, rake angle and Depth of cut are the input variables and cutting forces and surface finish are the output responses. In the present research paper four factors will be considered and each factor consists of five levels as shown in the Table 4.

Parameters	-2	-1	0	+1	+2
Cutting Speed(m/min)	65	85	105	125	145
Feed (mm/rev)	0.04	0.08	1.2	1.6	2.0
DOC(mm)	0.4	0.6	0.8	1.0	1.2
Rake Angle(Degree)	-10	-6	0	7	14

The design of experiments has a major effect on the number of experiments needed. Therefore it is essential to have a proper design of experiments. In order to reduce the number of experiments and resources such as time, material and money. The central composite design(CCD) technique is used. It reduced the number of experiments from 625 to 31 only. Experiment lay out along with the output response is shown in table 5.

S.No	Cutting Speed(v)	Feed(f)	DOC(t)	Rake Angle(0)	Cutting Force(N)	SurfaceRoughness(µ)
1	105	0.12	1.2	0	422	1.482
2	125	0.08	1	7	245	1.04675
3	125	0.08	1	0	275.2	0.48825
4	85	0.08	1	7	258.3	0.6816
5	85	0.16	1	-6	450.2	1.27255
6	85	0.08	1	-6	293	0.66645
7	85	0.16	1	7	440.1	0.912
8	125	0.16	1	7	401.3	1.2211
9	125	0.16	1	-6	450.7	1.1416
10	105	0.12	0.8	14	287.3	0.81425
11	105	0.12	0.8	0	321.1	0.5018
12	105	0.12	0.8	0	317.2	0.5018
13	65	0.12	0.8	0	360.1	0.4198
14	105	0.12	0.8	0	312.7	0.53525
15	105	0.04	0.8	0	170.2	0.3483
16	105	0.12	0.8	-10	308.1	0.61875
17	145	0.12	0.8	0	324	0.3972
18	105	0.12	0.8	0	316	0.38925
19	105	0.12	0.8	0	317.5	0.387
20	105	0.12	0.8	0	331	0.55735
21	105	0.12	0.8	0	330	0.37
22	105	0.2	0.8	0	433.8	0.43695
23	125	0.16	0.6	-6	279	0.9027
24	85	0.08	0.6	7	165.4	0.7557
25	85	0.16	0.6	7	274	0.4255
26	85	0.08	0.6	-6	179.9	0.82665
27	125	0.08	0.6	-6	194.3	0.26505
28	125	0.16	0.6	7	277.3	0.33645
29	125	0.08	0.6	7	164	0.81455
30	85	0.16	0.6	-6	279.2	0.66795
31	105	0.12	0.4	0	184.2	0.935

Table 5: Experiment lay out and output response

## 4. METHODOLOGY

The regression based models were developed by RSM to state the relationship between the input responses and output responses. The response surface graphs are generated with help of Design Expert software (trial version).

These graph are helpul to findout the value of process parameters as per the desired output quality. The response surface graph of the output responses with respect to input parameters are shown in figure. 2-13 The RSM based second order models have been found good for the optimization of variables for the responses. The statistical tool ANOVA is applied to check the model adequacy for the surface roughness and cutting force. Also the amount of contribution of each input process parameter for responses has been obtained. The surface roughness and cutting force both are desired to be minimum for the better quality of turned product. Fig. 2-7 were used to search the optimum value of process parameters for the minimum value of surface roughness. the parameters level have been identified are cutting speed 105 m/min, feed rate 0.08 mm/rev. rake angle 7 degree and depth of cut 0.4 mm. The statistic model in terms of coded value of factors for surface roughness is developed and found suitable for prediction. The equation model is as follows:

Surface Rouhness (Ra)= 5.99 - 0.0146 v - 17.39 f - 10.21 t - 0.0400 a + 0.00003 v \* v - 3.1 f \* f + 4.097t \* t + 0.002192 a \* a + 0.0627 v \* f + 0.00874 v \* t + 0.000693 v \* a + 16.89 f \* t 0.532 f \* a + 0.0351 t \* a



Fig.2. Surface plot of surface roughness vs Cutting Speed and Feed Rate.







Fig.4. Surface plot of surface roughness vs Cutting Speed and Rake Angle.

(1)







Fig.6. Surface plot of surface roughness vs Rake Angle and Feed Rate



Similarly cutting force is the second output response which also desired to be minimum for good quality of turning. The surface plots of cutting force are depicted in Fig. 8-13. From surface plots of cutting force, the level of parameters have been identified for minimum value of cutting force are cutting speed 125 m/min, feed rate 0.08 mm/rev. and depth of cut 0.6 mm and rake angle 7 degree. The statistic model in terms of coded value of factors for surface roughness is developed and found suitable for prediction. The equation model is as follows:

Cuting Force(Fy) =  $-178 - 0.09v + 1494f + 505t + 3.43\alpha + 0.00502v*v - 5002f*f - 193.2t*t - 0.2174$  $\alpha*\alpha - 2.17v*f - 1.170v*t - 0.0282v*\alpha + 1986f*t + 13.9f*\alpha - 4.10t*\alpha$ 



Fig.8. Surface plot of Cutting Force vs Cutting Speed and Feed Rate.



Fig 9. Surface plot of Cutting Force vs Cutting Speed and DOC.







Fig.11. Surface plot of Cutting Force vs Cutting Speed and Rake Angle.







Fig.13. Surface plot of Cutting Force vs Rake Angle and DOC.

The adequacy of established model for cutting force and surface roughness and cutting force has been checked at 95% confidence interval level using ANOVA respectively. The settled models were found good and suitable for prediction of the responses. The ANOVA table for the surface roughness and cutting force has been shown in table.5 and table.6 respectively. The R-square for surface roughness and cutting force are 0.8485 and 0.9833 respectively. The R-square value is a measure of variability in the observed response. The values of coefficient of determination R-square are nearly equal to 1, which confirmed that the developed models are acceptable.

Sourco	Sum of	đf	Mean	F	p-value	% of Contributi
Source	Squares	ui	Square	Value	Prob> F	on
Model	2.66	14	0.19	10.51	< 0.0001	
v	0.039	1	0.039	2.15	0.1623	1.32
f	4.22E-04	1	4.22E-04	0.023	0.8804	0.01
t	0.31	1	0.31	17.33	0.0007	10.5
α	0.28	1	0.28	15.74	0.0011	9.49
V*f	0.039	1	0.039	2.18	0.1595	1.32
V*t	0.019	1	0.019	1.06	0.3188	0.64
V*α	0.11	1	0.11	5.94	0.0268	3.73
f*t	0.28	1	0.28	15.72	0.0011	9.49
F*α	0.28	1	0.28	15.27	0.0013	9.49
t*α	0.03	1	0.03	1.66	0.2163	1.02
v^2	2.95E-05	1	2.95E-05	1.63E-03	0.9683	0
f^2	7.11E-04	1	7.11E-04	0.039	0.8452	0.02
t^2	1.13	1	1.13	62.81	< 0.0001	38.3
α^2	0.19	1	0.19	10.56	0.005	6.44
Residual	0.29	16	0.018			
Lack of Fit	0.25	10	0.025	4.09	0.0493	
Pure Error	0.037	6	6.17E-03			
Totall	2.95	30				
R-Squared	90.19		Adj R-Squared	80.61		

Table 5. ANOVA of Surface Roughness

Sauraa	Sum of	đf	Mean	F	p-value	% of
Source	Squares	ai	Square	Value	Prob> F	Contribution
Model	2.12E+05	14	15137.25	67.25	< 0.0001	
V	69.81	1	69.81	0.31	0.5853	0.28
F	1075.82	1	1075.82	4.78	0.044	4.29
Т	5902.89	1	5902.89	26.22	0.0001	23.5
А	149.47	1	149.47	0.66	0.4271	0.6
V*f	46.98	1	46.98	0.21	0.6539	0.19
V*t	342.29	1	342.29	1.52	0.2353	1.37
V*α	193.28	1	193.28	0.86	0.3679	0.77
f*t	3948.33	1	3948.33	17.54	0.0007	15.7
F*α	187.46	1	187.46	0.83	0.375	0.75
t*α	408.57	1	408.57	1.82	0.1967	1.63
v^2	115.7	1	115.7	0.51	0.4837	0.46
f^2	1834.52	1	1834.52	8.15	0.0115	7.32
t^2	1710.61	1	1710.61	7.6	0.014	6.83
α^2	1875.08	1	1875.08	8.33	0.0107	7.48
Residual	3601.4	16	225.09			
Lack of Fit	3300.13	10	330.01	6.57	0.0158	
Pure Error	301.27	6	50.21			
Total	2.16E+05	30				
R-Squared	98.33		Adj R-Squared	96.87		

Table 6. ANOVA of Cutting Force(Fy)

## **5. RESULT & CONCLUSION**

RSM was used to find the optimal level of variables for cutting force and surface roughness. In ANOVA, it has been discovered that the depth of cut has major physical as well as statistical influence on the surface roughness (10.51 %) right after the rake angle (9.49 %). It is because the workpiece and tool contact area is increased which direct effects the output response. Also the higher effect of interaction of cutting velocity and depth of cut has been found (9.49 %). Also the cutting force was influences by depth of cut (23.5%) then feed (4.2%). The highest interaction effect of feed and depth of cut on cutting force has been found (15.75%). Following points has been drawn on the bases of executed experiments and statistical results:

*a)* The optimal sets of cutting variables for better surface finish and minimum cutting force are determined.

*b)* Central composit design can be employed to develop mathematical models for predicting surface roughness and cutting force.

*c)* The RSM is found good for the searching of optimum value of parameteters, which has been confirmed through confirmatory experiment.

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# Second Law Efficiency and Exergy Destruction Analysis of Vapour Compression Refrigeration System

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## ABSTRACT

The paper presents the analysis of exergy for Vapour Compression Refrigeration System (VCRS) influenced by variation in evaporator temperature. The analysis of the processes and cycle is based on exergy destruction due to irreversibilities. The present work analyzed the behaviour of three refrigerants of Vapour Compression Refrigeration System (VCRS) with variation in evaporator temperature. The various parameters calculated are total irreversibility, second law efficiency. The primary objective of this paper is to analyze the system processes separately and to identify and quantify the sites having largest energy and exergy flow losses. In addition to this, the future prospects of the refrigerants have also been discussed.

.Keywords: Exergy destruction, second law efficiency

## **1. INTRODUCTION**

According to the thermodynamics principle, the heat transfer in air-conditioning takes place only at a finite temperature difference which is proportional to the heat transfer rate. The losses in the air-conditioning system need to be calculated by individual processes that make up the system. Energy analysis is the most commonly used method in the analysis of thermal systems, but it gives no indication about the degraded performance of system. Exergy shows that energy having quality as well as quantity, and actual processes occur in the direction of decreasing quality of energy. Energy analysis is concerned only with the conservation of energy, but exergy analysis shows directly the working efficiency.

An exergy analysis is usually aimed to determine the maximum performance of the system and identify the sites of exergy destruction. Exergy analysis of a refrigeration system can be performed by analyzing the components of the system separately. Identifying the main sites of exergy destruction shows the direction for potential improvements. An important object of exergy analysis for systems that consume work such as refrigeration is finding the minimum work required for a certain desired result. There have been several studies on the exergy analysis of refrigeration system and heat pump systems.

Journal of Dynamics of Fluids (Volume- 12, Issue - 1 January-April 2024 )

Refrigeration is the process of removing heat from an enclosed or controlled space, or from a substance, and moving it to a place where it is unobjectionable. The primary purpose of refrigeration is lowering the temperature of the enclosed space or substance and then maintaining that lower temperature as compare to surroundings. Cold is the absence of heat, hence in order to decrease a temperature, one "removes heat", rather than "adding cold."

The basic objective of developing a vapor absorption refrigerant system for automobile is to cool the space inside the automobile by utilizing waste heat and exhaust gases from engine. The air conditioning system of automobile in today's world uses "Vapor Compression Refrigerant System" (VCRS) which absorbs and removes heat from the interior of the automobile which is the space to be cooled and further rejects the heat to be elsewhere. Now to increase an efficiency of automobile beyond a certain limit vapor compression refrigerant system resists it as it cannot make use of the exhaust gases from the engine. In vapor compression refrigerant system, the system utilizes power from engine shaft as the input power to drive the compressor of the refrigerant system, hence the engine has to produce extra work to run the compressor of the refrigeration system utilizing extra amount of fuel.

VCRS	Vapour Compression Refrigerant System
COP	Coefficient of performance
Wc	Power input to the compressor (kW)
m	Mass flow rate of the refrigerant (kg/s)
Н	Specific Enthalpy (kJ / kg )
I <sub>12</sub>	Exergy destruction in compressor (kW)
S	Specific entropy (kJ/kg-K)
h	Actual specific enthalpy (kJ / kg )
s'	Actual specific entropy (kJ / kg -K)
E	Exergy (kW)
Г	Actual exergy destruction (kW)
W'e	Actual compression work or motor input
Т	Ambient temperature

#### Table 1: Nomenclature

#### 2.0. Literature Reviews

A literature review was conducted in the specific area of analysis related to VCRS using R-12, R-22 and R-134a. The literature available can be broadly classified as:

- Performance parameter
- Efficiency
- Exergy analysis

#### 2.1 Performance parameter:

Mahajan and Borikar found out that the performance of HC-12a in the domestic refrigerator condenser temperature and evaporator temperature, COP, refrigerating effect, condenser duty, work of compression and heat rejection of water are better than those of R134a throughout all the operating conditions. Venkataiah and Rao thermodynamically analysed R22, R134a, R404A, R407C, R410A, R507A, R290 and R600a using COOLPACK software .It focuses on fixed condenser temperature but with variable evaporator temperatures. Tashtoush et.al experimented on the replacement of R12 in domestic refrigerators by new hydrocarbon/hydrofluorocarbon refrigerant mixtures. The results show that butane / propane / R134a mixtures provide excellent performance parameters, such as coefficient of performance of refrigerator, compression power, volumetric efficiency, condenser duty, compressor discharge pressure and temperature, relative to a 210 g charge of R12. Fatouh and Murthy observed the Influence of operating temperatures at generator, absorber, condenser and evaporator on the performance of a single-stage vapour absorption refrigeration system (VARS) working with HCFC22-DMA, HCFC22-DMF and HCFC22-DMETEG pairs. Rocca and Panno presented the results of an experimental analysis comparing the performance of a vapour compression refrigerating unit operating with R22, and its performance in comparison to a new HFC fluid. Chakravarthy and Kumar intended to replace R-22 refrigerant by R-407C (mixture of R-32/125/134a), R-407A (mixture of R-32/125/134a) which better thermal properties and acceptable pressure and temperature ranges. Patel and Kapadia tested a vapour compression refrigeration (VCR) system with water cooled condenser and evaporator for simultaneous heating and cooling utilities. Experimental results show that R134a has good performance than R22 and performance of R407 is in same manner as R22.Vandaarkuzhali and Elansezhian did an experimental investigation to reduce the usage of R22 with the Hydrocarbon Refrigerant mixtures (HCM) of R22 and R152a refrigerants in the ratio of 30:70, 50:50, and 70:30 by mass. The overall performance of the system proved that the HCM could be a long term substitute for R22 (chlorodifluoromethane).

## 2.2 Efficiency:

Yadav and Nagalakshimi explore performance and efficiency variations of a refrigeration system using R12 and R134a refrigerant. Raja et.al did an analysis of energy and exergy on a traditional Vapor Compression Refrigeration Cycle using R152a, R290, R600, R600a, R123 and R717. The result deduced that these alternative refrigerant R600, R600a, R717 and R152a had higher COP and exergetic efficiency than R134a for evaporative temperature which range from 248 K to 283 K and condensation temperature 318 K with superheating 10 K and subcooling 5 K.

## 2.3 Exergy analysis :

Xu and Clodic introduced an exergy analysis method on Vapor Compression Refrigeration Cycle in order to compare the performance between 3 refrigerators using R12, R134a and R290 as the refrigerants. The refrigerator of R134a is almost efficient than for R12. But freezers for R134a and for R290 are less efficient than R12 freezer. Zakirov and Karimov evaluated the efficiency of evaporators with rolled-up pipes by the exergy analysis method. Reddy et.al did an exergy analysis of a Vapor Compression Refrigeration Cycle with selected refrigerants and found that R134a has the better performance in all respect, whereas R407C refrigerant has poor performance. Lee et.al presents numerical analysis of exergy for air-conditioning influenced by ambient temperature. The result shows that reducing exergy loss of the capillary influenced by the ambient temperature is the key for improving working efficiency of an air-conditioning system.

After reviewing it was found that there is a gap in work carried out in the field of total exergy destruction and second law efficiency and so it is proposed in this paper.

## 3.0 Methodology

There are three methodologies to evaluate exergy destruction and second law efficiency. These are :-

- Experimental method
- Simulation method
- Analytical method

In the present analysis we used analytical method using basis VCR system and exergy destruction formula to analyze exergy destruction and second law efficiency.

## 3.1 Cycle description:

The vapor compression refrigeration cycle is the majorly applied refrigeration cycle, which consists of a compressor, condenser, throttling device and an evaporator with controls and interconnections. Fig.1 exhibits the block diagram of a basic VCRS, which is a general irreversible cycle model.



The figure shows the different components of the vapour compression refrigeration cycle and the flow direction of the refrigerant cycle from the begin with suction of compressor, which is convenient to explain the procedure. In process, the refrigerant is firstly sucked and compressed by the compressor. At the exit of the compressor, refrigerant is with extremely high pressure and superheated. The compressed refrigerant will influx into the condenser to be condensed and takes place the heat exchange with the surroundings. The emitted heat of refrigerant during condensing in the condenser is transferred into the surroundings through the forced convection. The condensed refrigerant in the condenser outlet is direct lead to the inlet of the throttling device and runs through the throttle device into the evaporator. The process of the evaporation for refrigerant in the evaporator will receive heat from the cooling space. After the evaporation of refrigerant in the evaporator, the refrigerant vapour is sucked again by the compressor and built the refrigerant or cycle.

## 3.2 Refrigerant chosen and its properties:

For our analysis we have chosen 3 refrigerants namely:

- R-12
- R-134a
- R-22

## 3.2.1 R-12

- R-12 was the first fluorocarbon refrigerant developed and used commercially and is still a standard for comparing other refrigerant.
- It has many properties especially suitable for use in refrigeration, such as good stability, little effect on elastomer and plastics, good solubility in lubricating oil and a reasonable compression ratio.
- Non-flammability, low toxity, inertness and stability were also recognised as essential refrigerant property.

## 3.2.2 R-134a:

- HFC 134a is an Environment friendly refrigerant. It has no chlorine and hence zero ozone depletion potential.
- HFC 134a is widely used as a replacement for CFC 12. It is used in various applications, such as domestic, commercial and industrial refrigeration and air-conditioning.
- The performance characteristics of HFC134a are similar to those of CFC 12.

## 3.2.3 R-22

- R-22 is used in practically all residential and light commercial air conditioning and to some extent in large tonnage applications with centrifugal compressors. It is also used for some industrial low temperature and for medium and low temperature display cases in supermarkets.
- The refrigerating capacity when used in same compressor running at same speed is about 60% greater with R-22 than with R-12 at any evaporating temperature. However compressor discharge temperatures are much higher with R-22 than with R-12.

## 3.3 Exergy Analysis.

The Exergy analysis bases on the basic vapour compression refrigeration system shown in Fig. 1. Numerical Modulation discussed the complete system and its four main devices separately. The applied vapour compression refrigeration system is defined to fit the following five assumptions:

## 3.3.1 Assumptions:

These are the assumptions for the vapour compression refrigeration system :

- Steady state, steady flow operation.
- Negligible pressure drops in the evaporator, condenser, and intersections.
- Actual compression process.
- Isenthalpic expansion in expansion device.
- Negligible kinetic and potential energies.

Table 2 exhibits design parameters of the applied system. The efficiency of a vapour compression refrigeration cycle is indicated by the coefficient of performance (COP), which is defined by the amount of cooling energy per supplied work. The COP of a vapour refrigeration cycle is expressed as equation

## COP = Q / W

Where Q is Cooling Energy and W is work input.

Parameter	Value
Refrigeration capacity	3.51 kW
Condenser Temperature	313K
Evaporator Temperature Range	243K ~ 293K
Refrigerants	R-12, R-22, R-134a
Ambient Temperature	298K
Isothermal efficiency	85%
Mechanical efficiency	84%
Electrical efficiency	90%

Table 2 Design parameters of the applied vapour compression refrigeration system

## 4.0 Exergy Analysis:

Referring to the main cycle loop in Fig. 1 from the first law of thermodynamics and a general exergy relation for different cyclic processes can be written as equations given below :

Applying exergy balance equation

$$\begin{split} \dot{e}_{1} + \dot{w_{c}} &= \dot{e}_{2} + \dot{I}_{12} \\ \dot{I}_{12} &= (\dot{e}_{1} - \dot{e}_{2}) + \dot{w}_{c} \\ \dot{I}_{12} &= \dot{m}\{(h_{1} - h_{2}) + T_{o}(S_{2} - S_{1})\} + \dot{w}_{c} \\ \text{Since process is isentropic i.e.} \\ S_{1} &= S_{2} \\ \dot{I}_{12} &= \dot{m}(h_{1} - h_{2}) + \dot{w}_{c} \end{split}$$

Where,

 $\dot{w}_c$  is power input to the compressor (kW), m is mass flow rate of refrigerant (kg/s), h is enthalphy (kJ / kg ), T<sub>o</sub> is the ambient temperature (K),  $\dot{I}_{12}$  is exergy destruction in compressor (kW), S is the specific entropy (kJ/kg-K), For actual cycle,

For actual cycle,  $\begin{aligned} \eta_{iso} &= 0.85 \\ \eta_{mech} &= 0.84 \\ \eta_{elec} &= 0.9 \end{aligned}$ Considering mechanical and electrical exergy loss, 
$$\begin{split} \dot{I}_{(mech.elec)} &= \dot{w}'_e - \dot{w}_c \\ &= \dot{w}'_e - \eta_{mech} \cdot \eta_{elec} \cdot \dot{w}'_e \\ &= (1 - \eta_{mech} \cdot \eta_{elec}) \dot{w}'_e \end{aligned}$$
 
$$\begin{split} \dot{e}_1 + \dot{w}'_e &= \dot{e}'_2 + \dot{I}'_{12} \\ \dot{I}'_{12} &= (\dot{e}_1 - \dot{e}'_2) + \dot{w}'_e \\ \dot{I}'_{12} &= \dot{m}\{(h_1 - h'_2) + T_o(S'_2 - S_1)\} + \dot{w}'_e \end{split}$$

Where,

h' is actual enthalphy
S' is actual entropy
İ' is actual exergy destruction
w'<sub>e</sub> is actual compression work or motor input

4.2 Exergy of Condenser

 $\dot{e}_2 = \dot{e}_3 + Exergy$  due to the heat loss to the surrounding +  $\dot{I}_{23}$ 

Exergy due to the heat loss to the surrounding  $= Q_{c} (1 - T_{o}/T)$ Since the surrounding is assumed to be at dead state Therefore, T = T\_0 Exergy due to heat loss to the surrounding = 0  $\dot{I}_{23} = \dot{e}_{2} - \dot{e}_{3}$  $\dot{I}_{23} = \dot{m}\{(h_{2} - h_{3}) + T_{o}(S_{3} - S_{2})\}$ 

4.3 Exergy of Expansion valve

$$\begin{split} \dot{e}_3 &= \dot{e}_4 + \dot{I}_{34} \\ \dot{I}_{34} &= \dot{m}\{(h_3 - h_4) + T_o(S_4 - S_3)\} \end{split}$$

Since it is as isenthalpic process Therefore,  $h_3 = h_4$  $\dot{I}_{34} = \dot{m} T_o(S_4 - S_3)$ 

$$\begin{split} & 4.4 \ \text{Exergy of Evaporator} \\ & \dot{e}_4 + Q_e(1 - T_o/T_e) = \dot{e}_1 + \dot{I}_{41} \\ & \dot{I}_{41} = (\dot{e}_4 - \dot{e}_1) + Q_e(1 - T_o/T_e) \end{split}$$

Since,  $T_o > T_e$   $Q_e(1 - T_o/T_e) = -ve$ i.e. decrease in exergy of the system so we have to supply the external exergy in the form of compressor work.

Total exergy destruction (Itotaldest) is given by,

 $I_{total\ dest} = I_c + I_{cond} + I_{expn} + I_{evap}$  The second law efficiency of the system is the ratio of actual COP and ideal COP.

$$\eta_{II} = \frac{(COP)_{actual}}{(COP)_{ideal}}$$

 $(COP)_{ideal} = T_c/(T_c - T_e)$ 

 $(COP)_{actual} = Refrigeration capacity/\dot{w}'_{e}$ 

## 5.0 Results:

## 5.1 Result Table

Refrigerants	R-134a		R-	·12	<b>R-22</b>		
Temp.range $T_E \rightarrow T_C$ (K)	I <sub>total</sub> (Kw)	ηπ	I <sub>total</sub> (Kw)	ηπ	I <sub>total</sub> (Kw)	ηπ	
243→303	1.4516	0.5817	1.4099	0.6069	1.4461	0.6071	
253→303	1.2184	0.6175	1.1931	0.6382	1.2206	0.6354	
263→303	1.0268	0.6506	1.0107	0.6688	1.0301	0.6636	
273→303	0.8644	0.6839	0.8549	0.6992	0.8690	0.6909	
283→303	0.6736	0.7173	0.6685	0.7285	0.6778	0.71840	
293→303	0.42278	0.7502	0.4704	0.7518	0.4566	0.7448	

## **5.2** Variation of exergy destruction with Evaporator temperature

Fig 2. Variation of exergy destruction with Evaporator temperature

## 5.2 Variation of second law efficiency with Evaporator temperature.



Fig 3: Variation of second law efficiency with evaporator temp.

#### **6.0** Conclusion

As per the analysis, from the result it can be concluded that for the decrease in temperature difference between the condenser and evaporator or for the fixed condenser temperature and increase in evaporator temperature, there is a gradual decrease in exergy was found that the performance of these refrigerants are almost same with a little variation of R-12 and R-22 with R-134a but refrigerant R-12 and R-22 are highly toxic and damages environment. Thus we can replace it by R-134a.

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# Study of Fluoride level in the Ground Water of Western Uttar Pradesh (India)

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## ABSTRACT

The fluoride concentration in ground water was determined in western utter Pradesh India where it is the only source of drinking water. Various other quality parameters such as pH, Electrical conductivity, TDS, total hardness, calcium hardness, magnesium Hardness and fluoride were also measured. Ground water is a major source of drinking water in urban areas as well as in rural areas. More than 85% of the rural population uses ground water for domestic purposes. High fluoride contents in ground water leads a health threat to millions of people around the world. Fluoride has been known to be found most frequently in ground water of higher concentrations depending on the nature of rocks. Natural fluoride contents in ground water of the area. Thirteen samples were collected from different villages of the area. In the study area the maximum fluoride concentration in ground water was recorded (0.86-3.3) mg/l. Majority of the sample do not comply with Indian as well as WHO water quality standards. Overall water quality was found satisfactory for drinking purposes without any prior treatment except a few locations out of thirteen villages.

Key words: Ground water quality, Fluoride, health

## **1. INTRODUCTION**

Fluoride (F<sup>¬</sup>) is important for development of health and bones. Among the water quality parameters, fluoride ion exhibits unique properties as its concentration in optimum dose in drinking water is advantageous to health and if the concentration exceeds the limit 1.5 ppm, this affects the health <sup>(1)</sup>. High fluoride concentration in the ground water and surface water in many parts of the world is a case of great concern. Fluoride is an ardent mineral-seeker and it accumulates in large quantities in mineralized tissues like teeth and bones <sup>(2)</sup>. The main sources of fluoride in ground water are fluoride-bearing rocks such as fluorspar, fluorite, cryolite, fluoroapatitle and hydroxyapatite <sup>(3)</sup>. Also the content in ground water is a function of many factors such as availability and solubility of fluoride minerals velocity of following water, pH, concentration of calcium and bicarbonate ions in water <sup>(3)</sup>. Variation of ground water quality in an area is a function of physical and chemical parameters that are greatly influenced by geological formations and anthropogenic activities <sup>(4)</sup> Ahmad et al <sup>(5)</sup> have compared the results of

ground water in Rajshai city of Bangladesh with recommended limits suggested by world health organization. Knowledge in hydrochemistry is more important to assess the quality of ground water for understanding its suitability for various needs.

Water is an essential natural resource for sustaining life and environment that we have thought to be available in abundance and free gift of nature however chemical composition of surface water is one of the prime factors on which the suitability of water for domestic, industrial and agriculture purpose depends. Fresh water occurs as surface water and ground water, in this ground water contributes only 0.6% of the total water resources on earth. It is major and preferred source of drinking water in rural and urban areas particularly in India. Fluoride enters the body through water, food, industrial exposure, drugs, cosmetics, etc. but the drinking water is the major source (75%) of daily intake. Due to its strong electro negativity, fluoride is attracted to positively charged calcium in teeth and bones. Major health problems caused by fluorosis, teeth mottling, skeletal fluorosis and deformation of bones in children as well as adults. Excess fluoride affects plants and animals also. The effect on agriculture was also evident due to inhibition on plant metabolism leading to necrosis, needle scratch and tip burn diseases. In animals also prominent symptoms of fluorosis were observed. In human beings effect on dental and skeletal tissues (genu valgum) can occur in adolescents and young adults and even children under 10 year of age among communities exposed to high level of fluoride. It can interfere with carbohydrates, lipid, protein, vitamins, enzymes and mineral metabolism when the dosage is high. Skeletal deformation and wreaking of joints are typical form of fluoride at high level of fluoride intake. Fluoride is primarily execrated in urine. The severity of injury is determined by duration of fluoride exposure and concentrations in ground water in India very significantly. In some parts of India, fluoride levels are below 0.5 mg/L.

In this present study, the data pertaining to fluoride concentration in the ground water of the study area of western Uttar Pradesh, India is analyzed. A total 13 points belonging to western Uttar Pradesh, from Saharanpur to Ghaziabad district are included in this study. The water quality parameters are measured viz, pH, Electric Conductivity, (TDS) Total Dissolved Solids, (TH) Total Hardness,  $(Ca^{2+})$  Calcium,  $(Mg^{2+})$  Magnesium hardness,  $(Cl^{-})$  chloride, Dissolved (DO) Oxygen and  $(F^{-})$  Fluoride.

## 2.0 MATERIALAND METHODS

Samples of ground water have been collected form 13 identified villages of the study area in western Utter Pradesh from five different districts (Fig-1) during the year 2012. They were analyzed by using Auto chemistry system (960 Orion USA) employing the standard method (APHA, 1992).

Journal of Dynamics of Fluids (Volume- 12, Issue - 1 January-April 2024)

Hydrogen ion concentration (pH) and specific electrical conductivity (SEC) was measured using pH and Conductivity meter. Total dissolve solid (TDS) were measured by using TDS meter. Total alkalinity (TA) as CaCO<sub>3</sub>, carbonate ( $CO^{2^{-}}_{3}$ ) and bicarbonate ( $HCO^{-}_{3}$ ,) were estimated by titrating against standard HCl. Total hardness (TH) as CaCO<sub>3</sub>) was analyzed by complxometric titration method using standard EDTA solution as titrant. Magnesium ( $Mg^{2^{+}}$ ) was computed, taking the difference between Total Hardness and calcium hardness values. Fluoride ( $F^{-}$ ) was analyzed, using Auto chemistry system. All the parameters are expressed in milligrams per liter (mg/l).The values obtained are recorded in tabular form in Table-1.

<u>Table -1</u> <u>Ground water quality with reference to Fluoride to western Uttar Pradesh.</u>

						Total						
		Sample	Nature	pН	Electric	Dissolved	Total	Fluorid	Calcium	Magnesium	Total	Dissolve
S.N	Locations	No.	of		Cond.	Solids	Hardness	е	Hardness	Hardness	Alkalinity	Oxygen
			sources		(mg/l)	(TDS)	(TH)	(F <sup>-</sup> )	(Ca <sup>2++</sup> )	(Mg <sup>2++</sup> )	(TA)	(DO)
						(mg/l)	(mg/l)	(mg/l)	(mg/l)	(mg/l)	(mg/l)	(mg/l)
1	Khajnwar	R-1	TW	б.8	160	650	425	1.8	89	336	145	7.5
2	Beherki	<b>R-2</b>	HP	7.8	400	700	940	3.2	111	829	130	7.8
3	Santagarh	R-3	TW	7.9	170	780	236	2.1	49	187	115	8.2
4	Nanandi	R-4	HP	6.9	260	980	1265	1.2	135	130	512	7.0
5	Sadhuli Hariya	R-5	HP	7.2	180	880	1425	1.86	400	1025	480	6.8
6	Maheshpur	R-6	HP	7.5	185	770	514	150	250	264	218	7.6
7	Budhana	<b>R-</b> 7	TW	7.3	307	650	303	2.76	150	153	108	8.0
8	Chandangarhi	R-8	HP	б.8	160	380	326	.086	106	220	145	7.8
9	Atali	R-9	HP	7.7	280	480	1380	1.3	280	1100	655	6.8
10	Barnawa	R-10	HP	7.9	261	550	500	1.75	150	350	285	8.2
11	Surna	R-11	HP	6.7	220	1100	900	2.5	300	600	213	8.2
12	Daluhera	R-12	TW	7.5	151	900	700	3.1	220	480	204	7.6
13	Mohan Nager	R-13	HP	7.5	165	700	655	1.7	170	485	175	7.8

HP= Hand Pump, TW=Tube well



**Fig:-1.** Sampling location, R1-Khajawar; R2-Beherki; R3-Santagarh; R4-Nanandai; R5-Saghuli Hariya; R6-Maheshpur; R7-Budhana, R8-Chanddher; R9-Atali; R10 Barnawa; R11-Daluhera; R12-Surna; R-13-Mohan Nagar.

## **3.0 RESULT AND DISCUSSION**

The results of analytical parameters of ground water collected from the various locations in Table No.1 show extraordinary high values of maximum parameters. This is because of its occurrence in a thick clayey horizon which was considered freak saline pocket. The groundwater has pH in the range of 6.7-7.9, indicating an alkaline medium. According to the TDS classification the majority of the samples are with high TDS in the range of (380-1100). The Total Hardness (Calcium and Magnesium) varies from (303-1425) mg/L, belonging to "very hard" to hard category.

The relationship of Total Alkalinity to Total Hardness in the ground water suggests that the water have both carbonate hardness (CH) and non-carbonate hardness (NCH) with the corresponding concentrations of 115 - 655 and 303 - 1425 mg/l respectively. Dissolved oxygen contents of samples collected from different sides vary from 6.8 to 8.2 ppm. These values suggest that all samples are from organic impurities.

Based on the concentration of fluoride prescribed for drinking water standard (ISI, 2000), the investigation are classified into three category : low < 1.00 mg/l; moderate F with 1.2- 1.8 mg/l and High F 2.00-3.2 mg/L (Table-1). Fluoride level in water is normally controlled by the calcium and magnesium salts. Higher the values of calcium and magnesium, higher will be the presence of Fluoride ions. Rivers and lakes generally contain fluoride levels less than 0.5mg per liter, but ground water, particularly in volcanic or mountains areas can contain as much as 50 mg per liter. <sup>(10)</sup> When fluoride content exceeds 2.0 ppm, then brownish spots varying from small to large in size, can be seen on numerous teeth in the great majority of the members of the exposed community. When the fluoride contents more than 2.5 ppm the enamel loses its smoothness: signs of serious dental hyper-fluorosis. The symptoms of intoxication appeared in immigrants one to four year after their arrival. The finding that it takes one to four year for symptoms to manifest themselves is at variance of 30-40 years in an endemic area was required for a definite picture of skeletal fluorosis to develop. An exceptionally high content of water fluoride (2 -5 ppm), excessive heat ( $45^{\circ}$ C) and a poor state of nutrition, the diet being deficient in Ca & vitamin-C may be possible factor responsible for the early development of skeletal fluorosis Utter Pradesh.

Though the government is committed for the supply of safe drinking and potable water, the plans are yet to prove themselves practical. Many NG Os have come up in different part of country to provide fluorine free water in rural areas. Different de-fluorination techniques of ground water. Herbal and simple technique with the use of Soda lime, Bleaching powder and alum is recommended for the de-fluorination of ground water in the study area.

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# Urban Rain Water Harvesting – Need and Comprehensive Approaches

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## ABSTRACT

As the water crisis continues to become severe due to an increasing gap between water available for public use and water required, there is an immediate and critical need for reform in water management system and one such system is Rainwater Harvesting. Rainwater harvesting is the collection and storage of rainwater for reuse, rather than allowing it to run-off or go untapped post flowing through the sewerage system of the city. Rainwater can be collected from rooftops or paved areas and instead of personal use can also be redirected for groundwater recharge using a recharge pit, shaft or borehole. The harvested water can be used for gardens, irrigation, domestic use with proper treatment etc.

Some novel approaches of Rain Water Harvesting are now available e.g Sponge Cities, Rain Saucer, creating rain gardens, depaving, flooded forests. All these concepts focus on improving the chances of water percolating into the earth's surface and hence, naturally recharging the groundwater.

Keywords : Rainwater Harvesting, Sponge Cities, Rain Saucer, Approaches to Rainwater Harvesting.

## **1. INTRODUCTION**

Despite the fact that India is bestowed with seven major rivers and several tributaries and a welldefined monsoon, it is fast becoming (or has already become) a parched nation. This dry abyss is because of growing population, rapid urbanization and the notion that water is a renewable resource, without realizing that the "renewal" is a time bound process and can happen only at a certain pace. There is huge lack of awareness of the acute deficit amongst vast majority of the population, not only amongst the poor but also amongst the rich, in fact, especially amongst the rich. At the back of the lack of awareness, comes poor individual interest in contributing towards management of water resources. India has 2.4% of the world's total land area, 17.1% of world population and 4% of total water. India is ranked 132 in per capita water availability<sup>[1]</sup> Population in India has seen an exponential grown from 361 million in 1950 to 1210 million in 2010.<sup>[2]</sup> (Fig 1.0). Per capita water availability has gone down from 5200m<sup>3</sup> in 1951 to 1588m<sup>3</sup> in 2010 as compared to (Fig 2.0).

Journal of Dynamics of Fluids (Volume- 12, Issue - 1 January-April 2024 )

International norms would categorize a country as 'water stressed' at water less than 1700 m<sup>3</sup> per capita per year and 'water scarce' at water availability less than 1000 m<sup>3</sup> per capita per year. The per capita surface water availability has decreased from 2309m<sup>3</sup> in 1991 to 1902 m<sup>3</sup> in 2001 Projections indicate that the surface water availability per capita is likely to dip to 1401 m<sup>3</sup> and 1191 m<sup>3</sup> by the years 2025 and 2050, respectively<sup>[3]</sup>.

The percentage of urban population of the total population has increased from 18% in 1960 to 33% in 2015<sup>[4]</sup>. The per capita water demand increases with the increase in urbanization. As per Indian Standard: IS1172 (1993) - a minimum of 70 to 100 litres per capita per day may be considered just adequate for domestic needs of urban communities, apart from non domestic needs as flushing requirements.



Fig 1.0 Source: 1951\_Census\_of\_India#/media/File:India\_population\_increase.GIF



Fig 2.0 Source: Water Resources Information System of India

As a general rule the following rates per capita per day may be considered minimum for domestic and non domestic needs:

Table	1:	Per	Capita	Water	Demand
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	For communities with population up to 20 000 and without flushing system						
1)	a) water supply through standpost	40 lphd (Min)					
	b) water supply through house service connection	70 to 100 lphd					
2)	For communities with population 20 000 to 100,000 together with full flushing system	100 to 150 lphd					
3)	For communities with population above 100 000 together with full flushing system	150 to 200 lphd					

The value of water supply given as 150 to 200 litres per capita per day may be reduced to 135 litres per capita per day for houses for Lower Income Groups (LIG) and Economically Weaker Section of Society (EWS), depending upon prevailing conditions.<sup>[5]</sup>

India is bestowed with tropical monsoon climate which means that there is huge temporal and spatial variation in water availability. Recurring droughts and frequent floods are regular natural calamities. For example, average rainfall in Goa is as high as 3,005mm and that in West Rajasthan is as low as 313mm<sup>[3]</sup>

Anthropogenic changes such as deforestation, increased concretization has accelerated the run-off in cities. This also means that lesser and lesser water percolates into soil and meets the aquifers. When the land cannot absorb water at the same rate as that of rainfall, run off occurs, hence frequency of floods and water logging has gone up. Recent examples are flooding in Delhi, Gurgaon and Hyderabad<sup>[6]</sup>



Fig 3.0: Waterlogging in Gurgaon Source: ndtv.com

## 2.0. Approaches for Urban Rainwater Harvesting

Experience from existing or traditional techniques should lead us to suitable approaches for better management of run-off. Public appreciation of the existing crisis is vital to our embracing the solution and for projects to succeed. There are various approaches that aim to solve the primary reason of water not reaching the aquifer, while there are others that are based on intercepting and harvesting the water that falls as rainfall. There is also a scope of these approaches to be followed by individuals, groups or government bodies.

**Depaving** Impermeable surfaces that keep the water from percolating into earth need to be minimized. The first step in harvesting rainwater is retaining surfaces that allow water to percolate and recharge the aquifers. Alternatives for concrete could consist of wood chips, decomposed granite, un-mortared bricks etc. that allow the water to seep through<sup>[7][8]</sup>

Other simple approaches include

- Installing Rain Barrels down spout to collect all rainwater in a barrel without incurring huge expenditure. (Fig 4.0)
- Creating a Rain Garden where water collected from roof tops is diverted towards a garden where deep rooted plants are cultivated. This promotes percolation of water.<sup>[9]</sup>(Fig 5.0)



Fig 4.0 Rain Barrel Source: <u>www.esf.edu</u> **DOA: Sep 24, 2016** 



Fig 5.0 Rain Garden
Source: <u>http://www.enterprise.mtu.edu/</u> DOA Sep 24, 2016

Incentivizing and Enforcing Post generating awareness, the first step taken could be incentivizing general public to invest in rainwater harvesting systems. It could also be driven by enforcing policies. For example, post several years of water crisis and more than 1000 mm annual rainfall, in 2001, rainwater harvesting has been made mandatory in Chennai. Notification has been issued by Tamil Nadu government with amendments to Tamil Nadu District Municipalities Rule 1972 &Multistoried& Public Buildings Rules 1973 with provision for conservation of rainwater by implementation of RWH in all the existing and new buildings.[10] But it was never enforced with proper design and monitoring.

Creating Freshwater Flooded Forests (Fig 6.0) are forests which are inundated with freshwater, either permanently or seasonally. They normally occur along the lower reaches of rivers and around freshwater lakes. The main purpose of the rain water harvesting is to utilize the locally available rain water to meet water requirements throughout the year without the need of huge capital expenditure. This would facilitate availability of uncontaminated water for domestic, industrial and irrigation needs. Examples are Myristica swamp (Fig 6.0) and Nelapattu Bird Sanctuary (India)[11]



Fig 6.0: Myristica Swamp, India Source: <u>www.sciencepole</u>.com DOA: Sep 29, 2016

## 3.0 New Approaches

**RainSaucer** Instead of the rooftop acting as a catchment, RainSaucer, which is an upside down umbrella and collects water straight from the skies, hence reducing risk of contamination. This decreases the possibility for contamination and makes potable water for developing countries a potential application. The various advantages of a RainSaucer (Fig 7.0) are listed below:

- It is small enough to be deployed anywhere
- RainSaucer is removable and can be cleaned and stored when not in use i.e. outside of rainy season. This also reduces the chances of contamination.
- The system is cheaper and easier to maintain since the need for plumbing and construction is eliminated
- There isn't a pre requisite of an existing structure so, literally, anyone can start using it as their supply of clean water.



Fig 7.0 Rain Saucer Source: www.rainsaucer.com DOA Sep 24, 2016

It is a concept that is not yet popular in India, though it has great potential, as Rain water Harvesting has been made mandatory in 18 out of 28 Indian states with no real system in place.

**Sponge Cities** "A sponge city is one that can hold, clean, and drain water in a natural way using an ecological approach", says Kongjian Yu, the dean of Peking University's College of Architecture and Landscape Architecture<sup>[12].</sup> The basic concept of a Sponge city is that it should allow the surfaces to absorb as much water as possible during rainstorms. Currently, cities have been rendered impermeable by roads, pavements, high rises and water from rainfall mostly goes into the sewage drains. Instead, in a Sponge city, the freshwater eco systems (rivers, lakes, urban wetlands, gardens, parks etc.) are are regenerated and expanded. Water, when absorbed by soil is purified naturally and stored as groundwater. This reduces the risk of flooding as water is getting absorbed than running off, it also reduces the load on the sewerage system<sup>[1]</sup> "Sponge Cities" are cities with an infrastructure that collects excess rainfall and integrates flood control in urban planning. A "sponge city" will solve the problems

Journal of Dynamics of Fluids (Volume- 12, Issue - 1 January-April 2024)

of flooding and also help in reusing rainwater when there isn't enough water. Besides reducing losses caused due to flooding, it also has a potential to create investment opportunities as this transformation will require new engineering products technologies and upgraded infrastructure. <sup>[12][13][14]</sup>



Fig 8.0 Conceptual View of Sponge City Source: <u>http://www.caggregate.com/?tag=sponge-city</u> DOA Sep 24, 2016

China presented the concept of Sponge Cities at the second session of the World Future Council *Future of Cities Salons* series held in Beijing on 26th April 2016<sup>[1].</sup> The concept seeks to tackle the root cause which is of rapid urbanization and heavy concretization causing a reduction in infiltrated water and as a result, urban flooding is a common menace of large cities. There is, hence, reduced recycling of water; sponge cities aim to correct this balance and reduce flooding and act as a sink and source during periods of excessive rainfall and periods of high water demand<sup>[15]</sup>

China envisions that by taking steps towards improving water permeation into the soil, water detention and storage, reuse post purification, 70% of rain water can be absorbed and reused. The underlying objective is to reduce and reverse the impact of urban construction on the natural eco system.

China has laid down new standards for construction to be carried out in an integrated way. All new construction is supposed to adhere to the new standards – this applies to all urban districts, residential areas, industrial areas and development zones. Older towns will be renovated while focusing on solving problems related to water clogging, polluted water bodies and rainwater harvesting.

## 4.0 **Conclusion:**

Public participation in tapping into the rainwater is critical to the management, regeneration and expansion of our water resources. Several methods of rainwater harvesting ranging from simple to complex are available. A RWH system can be set up with minimal technical knowledge. There are several online communities and resources available for interested individuals and communities. Every drop harvested is a drop saved.

Rainwater harvesting can be an effective means of creating an independent water supply during local and regional water scarcity and if fully developed, can be used to supplement the main supply. It provides water when there is a famine or drought, can help mitigate flooding of low-lying areas, and reduces demand on groundwater usage. Other benefits include availability of water low in salinity, hence, reduced need for clean water in the public distribution system, lesser storm water load on sewerage system and lesser stormwater runoff polluting freshwater bodies.

Rainwater manipulated can not only reduce urban flooding but can also generate dry weather resource for the city. The amount of water that can be generated can be exemplified by a recent rainstorm in Delhi which recorded 82mm in a day. With an area of 1484km<sup>2</sup>, and percolation coefficient as 0.6, the total water available from this rainstorm event was sufficient to meet the per capita demand of 130 litres per day for the population of 25 million in Delhi<sup>[16]</sup> for 21 days!

It is clear that with numerous comprehensive approaches available, it is incumbent upon us that we take individual responsibility of water management and conservation, besides judicious use, in order to ensure clean water availability for all in the coming years

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# Microwave Assisted Rapid Synthesis of Some Schiff Bases and Their Antimicrobial Activity

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# ABSTRACT

A microwave promoted simple, clean and efficient synthesis of Schiff bases of 2-

hydroxybenzaldehyde and substituted 2–amino pyridine as precursors was done and its derivatives were prepared. Microwave reactions under solvent-free conditions or minimal solvent usage are attractive in offering reduced pollution, low cost and offer high yields together with simplicity in processing and handling. The isolated compounds obtained, were purified and characterized by IR and NMR spectral data and were subsequently subjected to the in-vitro antimicrobial activity against few pathogenic strains of microbes.

*Keywords:* Schiff base,2-hydroxybenzaldehyde, substituted 2–amino pyridine, microwave irradiation, antimicrobial.

## **1. INTRODUCTION**

Two third part of the entire organic compounds deals with heterochemistry. They have high synthesis flexibility, varied coordinating ability and medicinal utility. Condensation of a carbonyl compound with varied primary amine or amino compound with elimination of water molecule forms a weak basic compound known as imine or an anil or azomethine, which is commonly known as Schiff base<sup>1</sup>. These compounds have their own identity and importance in pharmaceutical, co-ordination and drug chemistry along with medicinal, biotechnological sciences<sup>2-3</sup> and hence it was thought interesting to investigate the reactions. Decent number of Schiff bases has been synthesized and reported for their bactericidal<sup>4-6</sup>, fungicidal<sup>7-8</sup>, antipyretic<sup>9-10</sup>, antitubercular<sup>11</sup>, antitumor<sup>12</sup> and anticancer activity<sup>13-14</sup>.

Synthesis of Schiff base is often carried out by acid-catalysis or generally by refluxing the mixture of aldehyde (or ketone) and amine in organic medium<sup>15-17</sup>. However, with the assistance of microwave irradiation, it was found that the condensation reaction could proceed fast and efficiently without solvent. The products could be purified simply by recrystallization in an appropriate solvent or a mixture of solvents with high yield of products. Thus microwave assisted reactions offers environmentally benign synthetic methods in terms of pollution, cost, yield and handling<sup>18-23</sup>.

Journal of Dynamics of Fluids (Volume- 12, Issue - 1 January-April 2024)

Synthetic route of Schiff base using 2-hydroxy benzaldehye and 2-amino pyridine by refluxing it conventionally in an acid catalysed organic medium has been reported by Asiri et-al<sup>15</sup>. However the present paper reports the synthesis of Schiff bases by the reaction of 2- hydroxybenzaldehyde and substituted 2–amino pyridine as precursors under microwave irradiations and its derivatives were then further studied for their antimicrobial potential. Structure of the synthesized compounds was confirmed by IR and <sup>1</sup>H-NMR spectroscopy. An enormous amount of work had been carried out and reported on Schiff bases showing Schiff base as promising microbial active agent<sup>24-28</sup>.

## 2. Materials and Methods

## Materials

The chemicals used for synthesis were of L.R. grade and purity of synthesized compounds was checked by TLC. All the working solutions were freshly prepared from the deionized water. To avoid any ionic contamination, deionized water was used for all the purpose in this study. The melting points of all synthesized compounds were recorded in precision digital melting point apparatus Model MP-D and are uncorrected. All experiments under microwave irradiation were carried out in unmodified domestic microwave oven model MC-7148MS manufactured by LG Electronics India Pvt. Ltd, Noida, India having maximum power output of 800W and 2450 MHz frequency. All the weighing was made on Citizen CY 104 one pan digital balance, ( $\pm$  0.0001gm). The IR spectrum of the synthesized compounds was recorded on Bruker Avance II 400 NMR spectrometer at Punjab University, Chandigarh.<sup>1</sup>H-NMR spectra were recorded on a Bruker Avance II 400 NMR spectrometer at Punjab University, Chandigarh in DMSO and CDCl<sub>3</sub> as a solvent and TMS as internal standard. Peak values are shown in d ppm.

The various microbial strains used in the study were *E. coli, S. typhi, S. paratyphi* and *S. aureus*. They were procured from M/s. Hi-Media Pvt. Ltd., Mumbai, India.

## Synthesis of Schiff bases under microwave irradiations

Equimolecular mixture of 2- hydroxybenzaldehyde and 2- aminopyridine in presence of catalytic amount of glacial acetic acid was taken in borosilicate glass beaker. The reaction mixture was then irradiated inside a microwave oven for 2 min at a power of P60. The reaction mixture was cooled and poured into ice cold water. Product formed, was separated by filtration and crystallized with alcohol to afford the title compound. The formation of ligand was confirmed by M. P and spectral studies.

Following is the scheme of the synthesis-



Thus with the substitution of  $R_1$  and  $R_2$ , following 8 Schiff bases were synthesised and screened for their antimicrobial activity against the above mentioned microorganisms.

- 1. N-(2'-hydroxybenzylidene) pyridine-2-amine  $(A_1)$
- 2. N-(2'-hydroxy-3'-nitrobenzylidene) pyridine-2-amine ( $B_1$ )
- 3. N-(2'-hydroxybenzylidene)-3-hydroxy pyridine-2-amine (A<sub>2</sub>)
- 4. N-(2'-hydroxy-3'-nitrobenzylidene)-3-hydroxy pyridine-2-amine (B<sub>2</sub>)
- 5. N-(2'-hydroxybenzylidene)-3-nitropyridine-2-amine (A<sub>3</sub>)
- 6. N-(2'-hydroxy-3'-nitrobenzylidene)-3-nitropyridine-2-amine (B<sub>3</sub>)
- 7. N-(2'-hydroxybenzylidene)-3-methylpyridine-2-amine (A<sub>4</sub>)
- 8. N-(2'-hydroxy-3'-nitrobenzylidene)-3-methylpyridine-2-amine (B<sub>4</sub>)

## 3. Result and Discussion

## Synthesized Schiff bases

The details of the substituted ligands synthesized under microwave irradiations are summarized in the following table. (2'-hydroxybenzylidene) pyridine-2-amine  $(A_1)$ 

Ligand	R1	R <sub>2</sub>	Molecular formula	Molecular weight	Colour	Melting point (°C)	Yield (%)	R <sub>f</sub> Value
A <sub>1</sub>	-H	-H	C <sub>12</sub> H <sub>10</sub> ON <sub>2</sub>	198	Yellow	63	83	0.68
A <sub>2</sub>	-H	-OH	$C_{12}H_{10}O_2N_2$	214	Crimson Brown	272	98	0.7
A3	-H	-NO2	C <sub>12</sub> H <sub>9</sub> O <sub>3</sub> N <sub>3</sub>	243	Pale Yellow	168	66	0.82
A4	-H	-CH3	C <sub>13</sub> H <sub>12</sub> ON <sub>2</sub>	212	Yellow	78	80	0.72
B1	-NO <sub>2</sub>	-H	$\mathrm{C}_{12}\mathrm{H}_9\mathrm{O}_3\mathrm{N}_3$	243	Amber	52	88	0.85
B <sub>2</sub>	-NO <sub>2</sub>	-OH	C <sub>12</sub> H <sub>9</sub> O <sub>4</sub> N <sub>3</sub>	259	Crimson Brown	258	92	0.88
B <sub>3</sub>	-NO <sub>2</sub>	-NO <sub>2</sub>	C <sub>12</sub> H <sub>8</sub> O <sub>5</sub> N <sub>4</sub>	288	Chrome Yellow	166	55	0.84
B4	-NO <sub>2</sub>	-CH3	C <sub>13</sub> H <sub>11</sub> O <sub>3</sub> N <sub>3</sub>	257	Yellow Ochre	66	61	0.86

## **Spectral Data Analysis**

- N-(2'-hydroxybenzylidene) pyridine-2-amine (A<sub>1</sub>) IR in cm<sup>-1</sup> (KBr pellets): 3001.43 (Ar-H str), 2976.44 (Ar-CH str), 3051.42 (Ar- OH str), 1453.17 (-C=N str (Schiff base)).
   <sup>1</sup>H-NMR (δ ppm): 13.45 (s, 1H, -OH str), 9.39 (s, 1H, -CH str), 6.89 to 8.47 (m, 8H, Ar-H str).
- 2) N-(2'-hydroxybenzylidene)-3-hydroxy pyridine-2-amine (A<sub>2</sub>) IR in cm<sup>-1</sup> (KBr pellets): 3165.10 (Ar-H str), 2972.34 (Ar-CH str), 3334.9 (Ar-OH str), 1455.9 (-C=N str (Schiff base)).
  <sup>1</sup>H-NMR (δ ppm): 13.102 (s, 1H, -OH str), 11.438 (s, 1H, -OH str), 8.70 (s, 1H, -CH str), 6.29 to 7.44 (m, 8H, Ar-H str).
- 3) N-(2'-hydroxybenzylidene)-3-nitropyridine-2-amine (A<sub>3</sub>) IR in cm<sup>-1</sup> (KBr pellets): 3091.99 (Ar-H str), 2919.05 (Ar-CH str), 3462.90 (Ar- OH str), 1431.88 (-C=N str (Schiff base)), 1331.22 (-C-NO<sub>2</sub> str).
  <sup>1</sup>H-NMR (δ ppm): 10.17 (s, 1H, -OH str), 8.37 (s, 1H, -CH str), 6.71 to 7.85 (m, 7H, Ar-H str).
- 4) N-(2'-hydroxybenzylidene)-3-methylpyridine-2-amine (A<sub>4</sub>) IR in cm<sup>-1</sup> (KBr pellets): 3046.39 (Ar-H str), 2973.36 (Ar-CH str), 3432.47 (Ar- OH str), 1452.9 (-C=N str (Schiff base)).
  <sup>1</sup>H-NMR (δ ppm): 13.75 (s, 1H, -OH str), 9.41 (s, 1H, -CH str), 6.91 to 8.32 (m, 7H, Ar-H str), 2.4337 (s, 3H, -CH<sub>3</sub> str).
- 5) N-(2'-hydroxy-3'-nitrobenzylidene) pyridine-2-amine (B<sub>1</sub>) IR in cm<sup>-1</sup> (KBr pellets): 3002.27 (Ar-H str), 2860.27 (Ar-CH str), 3052.26 (Ar- OH str), 1454.13 (-C=N str (Schiff base)), 1349.2 (-C-NO<sub>2</sub> str).
  <sup>1</sup>H-NMR (δ ppm): 13.45 (s, 1H, -OH str), 9.45 (s, 1H, -CH str), 6.9 to 8.48 (m, 7H, Ar-H str).
- 6) N-(2'-hydroxy-3'-nitrobenzylidene)-3-hydroxy pyridine-2-amine (B<sub>2</sub>) IR in cm<sup>-1</sup> (KBr pellets): 3072.28 (Ar-H str), 2855.43 (Ar-CH str), 3328.27 (Ar- OH str), 1454.29 (-C=N str (Schiff base)), 1338.34 (-C-NO<sub>2</sub> str).
  <sup>1</sup>H-NMR (δ ppm): 13.405 (s, 1H, -OH str), 11.207 (s, 1H, -OH str), 8.164 (s, 1H, -CH str), 6.81 to 7.49 (m, 6H, Ar-H str).

- 7) N-(2'-hydroxy-3'-nitrobenzylidene)-3-nitropyridine-2-amine (B<sub>3</sub>)
  IR in cm<sup>-1</sup> (KBr pellets): 3094.10 (Ar-H str), 2627.26 (Ar-CH str), 3277.19 (Ar- OH str), 1458.21 (-C=N str (Schiff base)), 1334.3 (-C-NO<sub>2</sub> str).
  <sup>1</sup>H-NMR (δ ppm): 10.45 (s, 1H, -OH str), 8.37 (s, 1H, -CH str), 6.72 to 8.23 (m, 6H, Ar-H str).
- 8) N-(2'-hydroxy-3'-nitrobenzylidene)-3-methylpyridine-2-amine (B<sub>4</sub>) IR in cm<sup>-1</sup> (KBr pellets): 3046.47 (Ar-H str), 2855.47 (Ar-CH str), 3338.51 (Ar- OH str), 1452.22 (-C=N str (Schiff base)), 1350.38 (-C-NO<sub>2</sub> str).
  <sup>1</sup>H-NMR (δ ppm): 13.74 (s, 1H, -OH str), 9.38 (s, 1H, -CH str), 6.9 to 8.31 (m, 6H, Ar-H str), 2.41 (s, 3H, -CH<sub>3</sub> str).

### **Antimicrobial Activity**

Schiff base compounds possess a wide range of biological activities which are associated with different substituents and the unsaturation of -C=N moiety in between the aryl rings. Hence, it is intended to examine their antimicrobial activities against their respective microbes-bacterial strains. For testing the antimicrobial activity, the compounds were assayed against *E. coli, S. typhi, S. paratyphi and S. aureus*. All these compounds were dissolved in DMSO and the ligand solutions were prepared with 20 mg/ml concentration. Gentamycin drug solution was used as the standard. The zone of inhibition was determined by disk diffusion method or zone inhibition method (ZIM) and minimum inhibitory concentration values (MIC values) were determined by serial dilution method.

#### Disk diffusion method

A 24 h fresh diluted culture of organisms under study was spread evenly over the entire surface of each petriplate containing solidified nutrient agar medium, using sterile cotton swab. Then the discs with 6mm diameter made up of Whatmann filter paper No.42, impregnated with the solution of the compounds (20mg/ml) was placed on the surface of inoculated plate. They were allowed to diffuse in the media and then the plates were incubated at 37°C for 24 h. The diameter of inhibition zone was observed and measured with the help of ruler<sup>29-30</sup>.

Table	1
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	Zone of inhibition (mm)						
Compounds	E. <i>coli</i>	S. typhi	S. paratyphi	S. aureus			
Gentamycin	46	46	49	38			
A <sub>1</sub>	8	6	4	6			
A <sub>2</sub>	5	6	5	10			
A <sub>3</sub>	18	16	14	12			
A4	6	8	10	13			
B1	20	24	11	16			
$B_2$	14	18	12	10			
B <sub>3</sub>	28	32	26	20			
B4	15	12	10	8			





#### Serial dilution method

The 5 ml of the nutrient broth medium was distributed in each sterile test tube. The 0.01 M stock solution of the test compounds, prepared in DMSO solvent was aseptically added to the various nutrient broth test tubes. Fresh culture of the test bacterium were inoculated in each test tube (0.2 ml culture) and were incubated at  $37^{\circ}$ C for 24 h and then were observed for minimum inhibitory concentration (MIC) against test bacterium<sup>31</sup>.

	Minimum inhibitory concentration (µg/ml)						
Compounds	E. coli	E. coli S. typhi S. paratyphi		S. aureus			
Gentamycin	300	650	1100	980			
A1	2000	1860	2180	1600			
A2	1400	900	980	1360			
A3	1200	980	1060	1140			
A4	1550	1320	1450	1660			
B1	1200	1280	1360	1400			
B2	1100	820	860	1140			
B3	900	860	940	1020			
B4	1300	960	1280	1250			

Table 1





From the table 1 and 2 above, it is evident that all the synthesized Schiff base compounds are biologically active against *E. coli*, *S. typhi*, *S. paratyphi and S. aureus*. Especially ligand B<sub>3</sub> had shown good activity against all the four pathogens.

Different substituents have different effects on the range of biological activities.  $-NO_2$  group being electron withdrawing is shown to enhance antimicrobial activity. Ligand B<sub>3</sub> containing two  $-NO_2$  groups shows highest value among all. Thus B<sub>3</sub>, B<sub>1</sub>, A<sub>3</sub> and B<sub>2</sub> have significant to moderate activity than A<sub>4</sub>, A<sub>2</sub> and A<sub>1</sub> due to presence of electron withdrawing nitro group. However, A<sub>4</sub> and B<sub>4</sub> has lower values of zone inhibition due to the presence of electron donating  $-CH_3$  group. Lower values for A<sub>2</sub> can be justified due to the presence of electron donating -OH group (Fig. 1 and 2).

## Conclusion

The present report gives the successful synthesis of the eight Schiff base ligands assisted by microwave irradiation which offers short reaction time, simplicity in handling, efficiency over conventional process and is a clean method. The synthesized compounds were purified and characterized by IR and NMR spectral data.

The antibacterial activity of all the synthesized ligands was studied and the data shows that both the methods – disk diffusion and serial dilution method gives comparable results of the ligands against pathogens under study.

Thus, the present study helps us to accomplish that ligand  $B_3$  and to some extent ligand  $B_1$ ,  $B_2$  and  $B_4$  show good activity against *E. coli, S. typhi, S. paratyphi and S. aureus* as compared to other synthesized ligands.

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