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Dr. (Lt.) R. K. Singh
Er. Manoj Kumar Sharma
Mr. Gyan Shekhar

Message



Dr. Anil Singh
Chancellor
Bhagwant University

I am pleased to know that the Faculty of Life Science & Applied Science is organizing a National Conference on “Future Innovation & Research in Science & Technology” on 1st March 2019.

Life Science and Applied Science is an expanding research field driven by Mathematics, Physics, Chemistry, Zoology Botany, and Environmental Science that eliminate old bottlenecks even as they create new challenges and opportunities for Life Science and Applied Science research.

The Conference theme is focused on Future Innovation and Research in both Science and Technology and also provides an opportunity to students to reflect their young minds in the area of research.

Speakers have assembled from different states and I take this opportunity to thank them for taking time out of their busy schedules for the conference.

I extend my good wishes and all success to the conference in achieving it's laid down objectives.

Dr. Anil Singh

Message



Dr. Asha Singh
Pro-Chancellor
Bhagwant University

It is my proud privilege to say that the Faculty of Life Science & Applied Science is organizing the National Conference “Future Innovation & Research in Science & Technology” on 1st March 2019.

The Conference provides a forum where the latest developments in the area of Pattern Recognition, Mathematics, Physics, Chemistry, Zoology, Botany and Environmental Science will be explored by many enthusiastic researchers.

I congratulate everyone who has contributed to this conference with their paper.

I express my hearty wishes for the shining success of this institution. Moreover, this whole event is a synchronized effort done by our faculties and students.

I wish all the best for success of the Conference.

Dr. Asha Singh

Message



Prof. (Dr.) V.K. Sharma
President/Vice-Chancellor
Bhagwant University

It is a matter of great pride that the Faculty of Life Science & Applied Science is organizing a National Conference on “Future Innovation & Research in Science & Technology” on 1st March 2019.

The goal of the Conference is to provide a forum for exchange of knowledge, experience, concerns and innovations among researchers, academicians and professionals in order to peep into the exciting and challenging future of Mathematics, Physics, Chemistry, Zoology, Botany and Environmental Science.

This Conference promotes in developing new strategy, adopting new Science and Technologies and provides the knowledge of the emerging trends in the field of Life Science & Applied Science. The Life Science & Applied Science not only encompasses the Mathematics, Physics, Chemistry, Zoology, Botany and Environmental Science but also penetrating every day into new sphere of human lives. This is creating economical and social impact on society.

The efforts of the faculty members and students of the Faculty of Life Science & Applied Science are commendable.

My heartiest congratulations to Dr. (Lt.) R. K Singh (Convener), Prof. R. K. Mathur, Er. Manoj Kumar Sharma (Co-Convener), Mr. Gyan Shekhar (Organizing Secretary), Mr. Bhanu Mathur, Ms. Kripa Sharma, Mr. Priyank Chaturvedi and Er. Manish Kumar Singh organizing committee members and technical committee for conducting this conference.

I wish them all the best.

Prof. (Dr.) V.K. Sharma

Bhagwant University, Ajmer

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Solve Some Transportation Problem Using Computational Techniques

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Abstract— In this article we are presenting some transportation problem using computational techniques. In this article we solve some transportation problem with the help of Computational Technique. The Computational Techniques method is better for solving Transportation Problem (TP). The model gives a very good result in Transportation problem (TP).

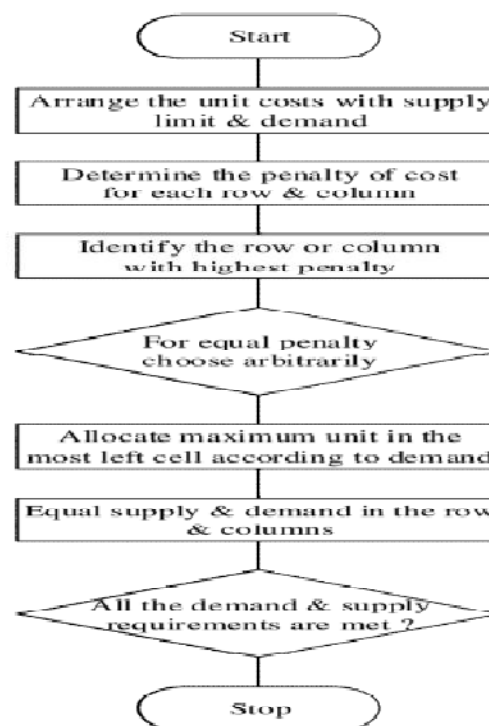
Keywords—computational; TP; Cost; Techniques;

I. INTRODUCTION

Transportation plays a leading role in the world financial system because the cost of transportation goes a long method in influencing the cost of finished products. That is the lower the transportation cost the cheaper the cost of products. This makes business organization, individuals and government to look for effective ways of solving transportation problems. From the discussion above one can easily come to the conclusion that the progress of any company is directly proportional to the efficiency of the transportation method of the company.

To solve a program for three methods of solving transportation problems. C++ was used to write the program on initial feasible solution and optimal solution using North West Corner Rule, Least Cost Rule and Vogel Approximation Method. From the result of the analysis, we discovered that the Programming on Vogel Approximation Method gives the same result at optimal solution and at low number of iterations. Hence we conclude that programming on Vogel Approximation Method is the best method of finding initial feasible solution, optimal solution and for distribution of good. Transportation is that the movement of individuals and commodities from one place to a different. The progress of any recent organization depends on the effective utilization of installation. Moreover, moving from one place to a different or distribution of products and services perpetually happen through installation. The transportation model depends on individual objectives and style in terms of price, safety, speed and comfortability [1],[4],[6].

| Sources | Supply Capacity |
|---------|-----------------|
| Plant 1 | 3,200 |
| Plant 2 | 3,080 |
| Plant 3 | 2,720 |
| Total | 9000 |



II. TRANSPORTATION PROBLEM

The following are three methods employed in establishing an initial feasible solution, they are a. North West Corner Method b. Least Cost Rule Method c. Vogel Approximation Method.

| | Methods (Programming) | Initial Feasible Solution | Optimal Solution | No of Iteration |
|----|------------------------|---------------------------|------------------|-----------------|
| 1. | North West Corner Rule | ₹1,427,360 | ₹1,288,480 | 6 |
| 2. | Least Cost Rule | ₹1,339,080 | ₹1,288,480 | 4 |
| 3. | Vogel Approximation | ₹1,295,080 | ₹1,288,480 | 2 |

III. A C PROGRAM TO IMPLEMENT TRANSPORTATION

PROBLEM

| | M ₁ | M ₂ | M ₃ | M ₄ | M ₅ | S _i |
|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| W ₁ | 150 | 165 | 150 | 145 | 100 | 3,200 |
| W ₂ | 148 | 162 | 172 | 127 | 150 | 3080 |
| W ₃ | 220 | 228 | 170 | 160 | 155 | 2,720 |
| d _j | 1,320 | 1,720 | 2,520 | 2,200 | 9000 | |

```
#include<stdio.h>
#include<conio.h>
main()
{
    int flag=0,flag1=0;
    int s[10],d[10],sn,cop=1,dm,a[10][10];
    int i,j,sum=0,min,x[10][10],k,fa,fb;

    clrscr();
    /* Getting The Input For the Problem*/

    printf("Enter the number of Supply\n");
    scanf("%d",&sn);
    printf("Enter the number of Demand\n");
    scanf("%d",&dm);
    printf("Enter the Supply Values\n");
    for(i=0;i<sn;i++)
        scanf("%d",&s[i]);
    printf("Enter the Demand Values\n");
    for(j=0;j<dm;j++)
        scanf("%d",&d[j]);
    printf("Enter the elements of the array\n");
    for(i=0;i<sn;i++)
    {
        for(j=0;j<dm;j++)
        {
            scanf("%d",&a[i][j]);
        }
    }
    /* Calculation For the Transportation */
    i=0;j=0;
    for(r=0;r<sn;r<dm;)
    {
        if(s[i]<d[j]) // Check supply less than demand
        {
            x[i][j]=a[i][j]*s[i]; // Calculate amount * supply
```

```
d[j]-d[j]; // Calculate demand - supply
i++; // Increment i for the deletion of the row
or
column
}
else if(s[i]>=d[j]) //Check the supply greater than equal to demand
{
    x[i][j]=a[i][j]*d[j]; // Calculate amount * demand
    s[i]=s[i]-d[j]; // Calculate supply - demand
    j++; // Increment j for the deletion of the row
or
column
}
}
/* The Cost Matrix is Estimated here */
printf("Given Cost Matrix is :
");
for(fa=0;fa<sn;fa++)
{
    for(fb=0;fb<dm;fb++)
    {
        printf("%d ",a[fa][fb]);
    }
    printf("\n");
}
/* The Allocated Cost Matrix is */

printf("Allocated Cost Matrix is
");
for(fa=0;fa<sn;fa++)
{
    for(fb=0;fb<dm;fb++)
    {
        printf("%d ",x[fa][fb]);
        sum=sum+x[fa][fb];
    }
    printf("\n");
}
/* Transportation Cost Estimated and Sum is Printed*/
printf("The Transportation cost:%d",sum);
getch();
}
```

IV. CONCLUSION

Since program industrial on Vogel Approximation has the benefits of getting initial possible solution; simple to work out and straightforward to edit once error are committed within the method of knowledge coming into. Therefore programming developed on Vogel Approximation methodology exploitation C is that the best methodology of obtaining Approximate answer to transportation drawback and best methodology of distributing the products and services.

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A Software Oriented Approach to Solve Some Transportation Problem Using Computational Performance and Techniques

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Abstract— In this paper we are presenting a software approach to solve some transportation problem using computational performance and techniques. In this paper we are solve some transportation problem with the help of C++ and Matlab. The MATLAB coding method is better than analytical method for solving Transportation Problem (TP). The model give a very good result in Transportation problem (TP).

Keywords—TP; Matlab; C++; Method; Analytic

1. INTRODUCTION

It is developed and published by Harold W.Kuhn(1995), who gave the name "Hungarian Method" because the algorithm was largely based on the earlier works of two Hungarian Mathematicians: Denes Konig and Jeno Egervary. Moreover MATLAB is a software package. MATLAB stands for MATrix LABoratory, it deals with matrix (array).

Now days MATLAB is very mostly used mathematics such as MATLAB with Differential Equation, Numerical methods, Operation Research, Fuzzy Logic etc. In this paper MATLAB coding is used to solve Transportation Problem. This gives optimal solution within fraction of seconds.

The Transportation drawback involves finding the lowest-cost arrange for distributing stocks of products or provides from multiple origins to multiple destinations that demand the products. The transportation model may be want to determine a way to portion the provides on the market from the assorted factories to the warehouses that stock or demand those product, in such some way that total shipping price is reduced. Usually, analysis of the matter can manufacture a shipping arrange that pertains to a precise amount of your time (day, week), though once the arrange is established, it will generally not amendment unless one or additional of the parameters of the matter (supply, demand, unit shipping cost) changes.

The transportation model starts with the event of a possible answer, that is then consecutive tested and improved till a best answer is obtained. The outline of the technique on the subsequent pages focuses on every of the most important steps within the method during this order:

II TRANSPORTATION PROBLEM (MATLAB PROGRAM)

```
function [x,cost]=transport(s,d,c);
% [x,cost]=transport(s,d,c)
% Input:
% s = supplies (m*1)
% d = demands (n*1)
% c = costs (m*n)
% Output:
% x = optimal solution (m*n)
% cost = minimal transport cost
```

```
function [x,b]=northwest(s,d)
% [x,b]=northwest(s,d)
% x: shipments using nwrule
(m*n)
% b: 1 for each basic variables 0 for nonbasic (m*n)
% s: supplies (m*1)
% d: demands (n*1)
if (sum(s)~=sum(d)),
disp('ERROR The total supply is not equal to the total demand'),
return;
end
m=length(s);
n=length(d);
i=1;
j=1;
x=zeros(m,n);
b=zeros(m,n);
while ((i<=m) & (j<=n))
if s(i)<=d(j)
x(i,j)=s(i);
b(i,j)=1;
d(j)=d(j)-s(i);
i=i+1;
else
x(i,j)=d(j);
b(i,j)=1;
s(i)=s(i)-d(j);
j=j+1;
end
```

```
end
end
example511; [x cost] = transport(s,d,c)
x =
```

```
    100    0    20    0
     0    60    60    20
     0     0     0   100
```

```
cost =
    1900
```

```
example513; [x cost] = transport(s,d,c)
x =
```

```
     0     0     0    30    70
    20    60    80     0     0
    30     0     0    70     0
```

```
cost =
    1730
```

III. PSEUDO CODE FOR THE TRANSPORTATION PROBLEM IS WRITTEN IN MAT LAB

| Items | Destination | | | | | Demand |
|--------|-------------|--------------|-------------|-------------|------------|--------|
| | A | B | C | D | E | |
| F | 7000 6 | 2000 | 6000 | 11000 | 90000 | 6 |
| G | 4000 94 | 5000 6 | 12000 | 8000 | 22000 | 100 |
| H | 9000 | 14000 194 | 21000 6 | 13000 | 19000 | 200 |
| I | 1000 0 | 18000 | 17000 44 | 25000 6 | 27000 | 50 |
| J | 3000 | 20000 | 26000 | 20000 94 | 28000 6 | 100 |
| Supply | 100 | 200 | 50 | 100 | 6 | 456 |

The total transportation cost is given as
 $7000*6+4000*94+5000*6+14000*194+21000*6+17000*44+25000*6+20000*94+28000*6= 62,36,000$

```
clc;
clear all;
close all;
x=input('enter the transportation matrix');
[m n]=size(x);
x1=zeros(m,n);
sumc=0;
sumr=0;
```

```
for i=1:m-1
sumc=sumc+x(i,n);
end
for j=1:n-1
sumr=sumr+x(m,j);
end
if(sumc == sumr)
for i=1:m
for j=1:n
x11=min(x(i,n),x(m,j));
x1(i,j)=x11;
x(i,n)=x(i,n)-x11;
x(m,j)=x(m,j)-x11;
end
end
else disp('unbalanced transportation');
end
xre=0;
for i=1:m-1
for j=1:n-1
xre=xre+(x(i,j). *x1(i,j));
end
end
disp(['the transportation cost is ',num2str(xre)]);
```

IV. CONCLUSION

It is a novel approach to solve the TP. We use MATLAB software to solve the transportation problems. It is very simple code write in Mat lab and this is a very simple programming languages. Transportation problem solve very easy through Matlab programming and results are very accurate. The system developed in this study was desktop-based which is limited to usage by only users who have the software installed on their computers. It will however be of more advantage if the system is made webbased as this will enable different users access the system from different locations and with different devices.

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An Introduction of Spectral theory of two-point ordinary differential operators

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Abstract— In this paper we are presenting an introduction of spectral theory of two point ordinary differential operator. In this article we are show some definition of spectral theory and its uses.

Keywords—Two point; Spectral Theory; Operators

I. INTRODUCTION

Spectral methods permeate the theory of partial differential equations. One solves linear PDEs by separation of variables, getting eigenvalues when the spectrum is discrete and continuous spectrum when it is not. Linearized stability of a steady state or traveling wave of a nonlinear PDE depends on the sign of the first eigenvalue, or on the location of the continuous spectrum in the complex plane. This minicourse aims at highlights of spectral theory for self adjoint partial differential operators, with a heavy emphasis on problems with discrete spectrum.

In the 1920s John von Neumann established a general spectral theorem for unbounded self-adjoint operators, which Kunikida Kodaira used to streamline Weyl's method. Kodaira also generalised Weyl's method to singular ordinary differential equations of even order and obtained a simple formula for the spectral measure. The same formula had also been obtained independently by E. C. Titchmarsh in 1946 (scientific communication between Japan and the United Kingdom had been interrupted by World War II). Titchmarsh had followed the method of the German mathematician Emil Hilb, who derived the eigenfunction expansions using complex function theory instead of operator theory. Other methods avoiding the spectral theorem were later developed independently by Levitan, Levinson and Yoshida, who used the fact that the resolvent of the singular differential operator could be approximated by compact resolvents corresponding to Sturm-Liouville problems for proper subintervals. Another method was found by Mark Grigoryevich Krein; his use of *direction functionals* was subsequently generalised by Izrail Glazman to arbitrary ordinary differential equations of even order.

The spectral theory of ordinary differential equations is the part of spectral theory concerned with the determination of the spectrum and eigenfunction expansion associated with a linear ordinary differential equation. In his paper Hermann Weyl

generalized the classical Sturm Liouville theory on a finite closed interval to second order differential operators with singularities at the endpoints of the interval, possibly semi-infinite or infinite. Unlike the classical case, the spectrum may no longer consist of just a countable set of eigenvalues, but may also contain a continuous part. In this case the eigenfunction expansion involves an integral over the continuous part with respect to a spectral measure, given by the Titchmarsh-Kodaira formula. The theory was put in its final simplified form for singular differential equations of even degree by Kodaira and others, using von Neumann's spectral theorem. It has had important applications in quantum mechanics, operator theory and harmonic analysis on semisimple Lie groups. Spectral theory for second order ordinary differential equations on a compact interval was developed by Jacques Charles François Sturm and Joseph Liouville in the nineteenth century and is now known as Sturm-Liouville theory. In modern language it is an application of the spectral theorem for compact operators due to David Hilbert. In his paper, published in 1910, Hermann Weyl extended this theory to second order ordinary differential equations with singularities at the endpoints of the interval, now allowed to be infinite or semi-infinite. He simultaneously developed a spectral theory adapted to these special operators and introduced boundary conditions in terms of his celebrated dichotomy between *limit points* and *limit circles*.

II. SPECTRAL THEORY OF TWO-POINT ORDINARY DIFFERENTIAL OPERATORS

Birkhoff systematically developed the spectral theory of two-point differential operators.

Stone extended Birkhoff's theorems on continuous functions onto the more modern Sobolev space. The principal references for regular problems and the more recent which uses the theory of Fredholm operators to improve upon the treatment of Dunford & Schwartz in several aspects. Irregular boundary conditions are comparatively less studied. Second order problems were first investigated by Stone, who derived their characteristic determinant. The completeness of the eigenfunctions of many such operators was established by

Yakubov but Lang and Locker showed that it does not hold for general second order irregular operators.

Locker's more recent monograph concentrates on simply irregular operators, finding eigenvalues and their multiplicities, and showing that the eigenfunctions are a complete system in L^2 . The third class, the degenerate irregular operators, is largely unstudied. One of the most fundamental theorems in the spectral theory of two-point ordinary differential operators is that the eigenvalues are precisely the zeros of the characteristic determinant, a function defined in terms of the boundary conditions. As the characteristic determinant is an exponential polynomial the theory of the distribution of the zeros of such functions is of great importance. We prefer Langer's papers to the more general, but considerably more dense, book of Levin as the former focus on finite sums instead of infinite series.

III. SPECTRAL OPERATOR

In mathematics, spectral theory is an inclusive term for theories extending the eigenvector and eigenvalue theory of a single square matrix to a much broader theory of the structure of operators in a variety of mathematical spaces.[1] It is a result of studies of linear algebra and the solutions of systems of linear equations and their generalizations.[2] The theory is connected to that of analytic functions because the spectral properties of an operator are related to analytic functions of the spectral parameter.[3]

The name spectral theory was introduced by David Hilbert in his original formulation of Hilbert space theory, which was cast in terms of quadratic forms in infinitely many variables. The original spectral theorem was therefore conceived as a version of the theorem on principal axes of an ellipsoid, in an infinite-dimensional setting. The later discovery in quantum mechanics that spectral theory could explain features of atomic spectra was therefore fortuitous. Hilbert himself was surprised by the unexpected application of this theory, noting that "I developed my theory of infinitely many variables from purely mathematical interests, and even called it 'spectral analysis' without any presentiment that it would later find application to the actual spectrum of physics." [4]

There have been three main ways to formulate spectral theory, all of which retain their usefulness.[clarification needed] After Hilbert's initial formulation, the later development of abstract Hilbert space and the spectral theory of a single normal operator on it did very much go in parallel with the requirements of physics; particularly in the hands of von Neumann.[5] The further theory built on this to include Banach algebras, which can be given abstractly. This development leads to the Gelfand representation, which covers the commutative case, and further into non-commutative harmonic analysis.

The difference can be seen in making the connection with Fourier analysis. The Fourier transform on the real line is in one sense the spectral theory of differentiation qua differential operator. But for that to cover the phenomena one has already to deal with generalized eigenfunctions (for example, by means of a rigged Hilbert

space). On the other hand it is simple to construct a group algebra, the spectrum of which captures the Fourier transform's basic properties, and this is carried out by means of Pontryagin duality.

One can also study the spectral properties of operators on Banach spaces. For example, compact operators on Banach spaces have many spectral properties similar to that of matrices.

The background in the physics of vibrations has been explained in this way:[6]

“ Spectral theory is connected with the investigation of localized vibrations of a variety of different objects, from atoms and molecules in chemistry to obstacles in acoustic waveguides. These vibrations have frequencies, and the issue is to decide when such localized vibrations occur, and how to go about computing the frequencies. This is a very complicated problem since every object has not only a fundamental tone but also a complicated series of overtones, which vary radically from one body to another. ”

The mathematical theory is not dependent on such physical ideas on a technical level, but there are examples of mutual influence (see for example Mark Kac's question Can you hear the shape of a drum?). Hilbert's adoption of the term "spectrum" has been attributed to an 1897 paper of Wilhelm Wirtinger on Hill differential equation (by Jean Dieudonné), and it was taken up by his students during the first decade of the twentieth century, among them Erhard Schmidt and Hermann Weyl. The conceptual basis for Hilbert space was developed from Hilbert's ideas by Erhard Schmidt and Frigyes Riesz.[7][8] It was almost twenty years later, when quantum mechanics was formulated in terms of the Schrödinger equation, that the connection was made to atomic spectra; a connection with the mathematical physics of vibration had been suspected before, as remarked by Henri Poincaré, but rejected for simple quantitative reasons, absent an explanation of the Balmer series.[9] The later discovery in quantum mechanics that spectral theory could explain features of atomic spectra was therefore fortuitous, rather than being an object of Hilbert's spectral theory.

Consider a bounded linear transformation T defined everywhere over a general Banach space. We form the transformation:

$$R_{\zeta} = (\zeta I - T)^{-1}$$

Here I is the identity operator and ζ is a complex number. The inverse of an operator T , that is T^{-1} , is defined by:

$$TT^{-1} = T^{-1}T = I$$

If the inverse exists, T is called regular. If it does not exist, T is called singular.

With these definitions, the resolvent set of T is the set of all complex numbers ζ such that R_{ζ} exists and is bounded. This set often is denoted as $\rho(T)$. The spectrum of T is the set of all

complex numbers ζ such that R_ζ fails to exist or is unbounded. Often the spectrum of T is denoted by $\sigma(T)$. The function R_ζ for all ζ in $\rho(T)$ (that is, wherever R_ζ exists as a bounded operator) is called the resolvent of T . The spectrum of T is therefore the complement of the resolvent set of T in the complex plane.[10] Every eigenvalue of T belongs to $\sigma(T)$, but $\sigma(T)$ may contain non-eigenvalues.[11] This definition applies to a Banach space, but of course other types of space exist as well, for example, topological vector spaces include Banach spaces, but can be more general.[12][13] On the other hand, Banach spaces include Hilbert spaces, and it is these spaces that find the greatest application and the richest theoretical results.[14] With suitable restrictions, much can be said about the structure of the spectra of transformations in a Hilbert space. In particular, for self-adjoint operators, the spectrum lies on the real line and (in general) is a spectral combination of a point spectrum of discrete eigenvalues and a continuous spectrum.[15]

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A Study of Covalency in Neodymium, Leucine and Urea & Thiourea in Molar Ratio 1:2:1

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Abstract: Neodymium an element of inner transition series(4f).The optical absorption spectra of Neodymium in leucine as primary ligand and Urea or Thiourea as secondary ligand are prepared in molar ratio 1:2:1.Spectral line of the solution lies in the visible range of 380nm to 900nm, recorded by UV-VS spectrometer 3000⁺.With the help of energy parameters, Structure and bonding of complexes have been studied. Nephelauxetic ratio are calculated. The electronic spectra of rare earths, both in natural and free ion states consists of closely spaced group ($\approx 10^2$ - 10^3 cm⁻¹) of sharp lines in the near infrared, visible, and ultraviolet region. They undergo modifications when the rare earth ions are placed in different lattice sites in crystals or different environments.

Key words- *Nephelauxetic Ratio, Bonding parameter, Neodymium, Leucine,Urea, Thiourea, UV-VS spectrometer.*

I. I. INTRODUCTION

Last seventy years, Lanthanides have gained much importance and have drawn the attention of researchers in Physical and chemical sciences[1-15]. Absorption spectra of Neodymium have been studied in its ternary complexes. Much work has been done on rare-earth with oxygen and carboxylic acids. Different ternary complexes of Neodymium with amino acid as primary ligand and urea or thiourea as secondary ligands are prepared in alcohol. Rare-earth complex usually do not form good single crystals and also decomposes in glassy matrix. A general theory of the solvent effect on the intensities of f-f transitions of lanthanide complexes, based on the static and dynamics coupling between metal ion ligand and solvent molecules will be discussed. Different parameters Slater-Condon parameters, Energy levels are calculated and compared with standard one.

Knowledge of rms deviation, nature of complex formation is determined. Strength of bonding helps to tell about the type of bonding between metal and ligands. Lanthanides have much importance due to their use as laser materials.

II. EXPERIMENTAL DETAILS

Neodymium in this experiment are 99.9% pure.All reagents used in this studied are taken to be of standard purity. In this work all chemicals are taken from C.D.H company. The complex will be synthesized with Leucine as primary ligand and Urea or Thiourea as secondary ligand molar ratios 1:2:1. The solution is stirred for half an hour with magnetic stirrer method. The absorption spectra of the complexes is recorded with UV-VIS Spectrophotometer LABINDA 3000⁺. Peaks of these absorption spectra are recorded in between400nm to 800nm.

III. PARAMETERS

Different parameters such as Slater Condon Parameters, bonding parameter $b^{1/2}$, the covalency of the complex will be calculated. The calculated energy levels parameters will be compared with the experimentally observed energy levels in different environments.

The energy levels of various transitions will be taken experimentally as well as theoretically by using Taylor Series expansion in first order approximation..

$$E_j(F_k, \xi_{4f}) = E_0(F_k, \xi_{4f}) + \sum \partial E_j / \partial F_k \Delta F_k + \partial E_j / \partial \xi_{4f} \Delta \xi_{4f}$$

Where $k = 2, 4, 6$

The values of F_2 , F_4 , and F_6 parameters will be computed using Judd-Ofelt relation and will be arranged in Tabulated form. The values of reduced matrix elements will be collected from W.T. Carnall. The parameter $b^{1/2}$ is a measurements of

types of bonding will be calculated by the given formula

$$b^{1/2} = [(1-\beta)/2]^{1/2}$$

Table-1 Energy levels of Neodymium Complexes
ND: LU: U (1:2:1)

ND: LU:TU (1:2:1)

| Levels | Observed energy | Calculated energy | Delta E | Observed energy | Calculated energy | Delta E |
|--------------------------------|-----------------|-------------------|---------|-----------------|-------------------|---------|
| ⁴ F _{3/2} | 11547.34 | 11541.68 | 5.66 | 11547.34 | 11552.6 | 24.73 |
| ⁴ F _{5/2} | 12578.61 | 12560.58 | 18.03 | 12578.61 | 12557.42 | 21.19 |
| ⁴ F _{7/2} | 13495.27 | 13397.57 | 97.70 | 13495.27 | 13382.83 | 112.43 |
| ⁴ F _{9/2} | 14705.88 | 14781.83 | -75.94 | 14705.88 | 14761.86 | -55.98 |
| ⁴ G _{3/2} | 17272.15 | 17365.79 | -93.63 | 17301.03 | 17367.13 | -66.10 |
| ⁴ G _{7/2} | 19157.08 | 19156.88 | 0.27 | 19157.08 | 19184.86 | -27.77 |
| ⁴ G _{9/2} | 19531.12 | 19554.49 | -23.37 | 19531.12 | 19588 | -56.88 |
| ² G _{7/2} | 21008.4 | 20988.45 | 19.95 | 21051.63 | 21021.64 | 30.99 |
| ⁴ C _{11/2} | 21691.97 | 21660.31 | 31.66 | 21646.02 | 21666.29 | -20.26 |
| ² P _{1/2} | 23364.48 | 23358.79 | 5.68 | 23041.47 | 23045.27 | -3.79 |
| rms deviation | | | 45.54 | | | 46.38 |

Parameters of Nd:Lu:U

ENERGY PARAMETERS

E1 : 5095.69

E2 : 26.43509

E3 : 495.0204

E1 / E3 : 10.2939

E2 / E3 : 5.340203E-02

F PARAMETERS

F2 : 340.9793

F4 : 47.26246

F6 : 5.531981

Zeta4F : 876.9626

F4 / F2 : .138608

F6 / F2 : .0162238

rms Deviation : 51.58042

Nephelauxetic Ratio : 1.029651

Bonding Parameter : .1217605

Parameters of Nd:Lu:TU

ENERGY PARAMETERS

E1 : 4984.662

E2 : 24.63476

E3 : 495.4134

E1 / E3 : 10.06162

E2 / E3 : 4.972566E-02

F PARAMETERS

F2 : 332.309

F4 : 48.88047

F6 : 5.149317

Zeta4F : 874.4746

F4 / F2 : .1470934

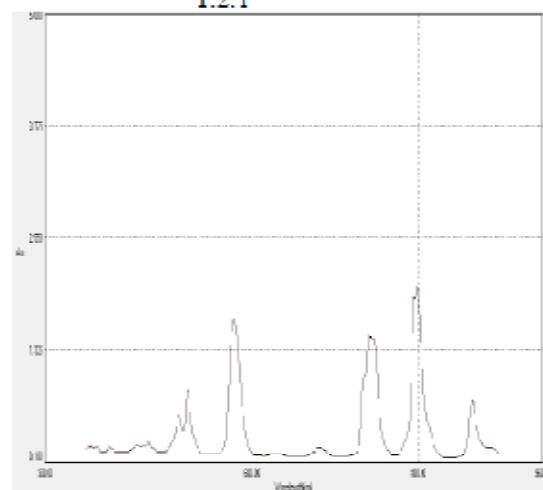
F6 / F2 : 1.549557E-02

rms Deviation : 51.57473

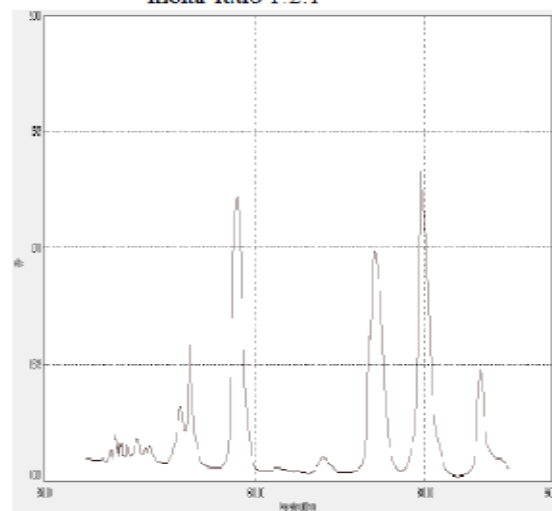
Nephelauxetic Ratio : 1.00347

Bonding Parameter : 4.165157E-02

Absorption Spectra of
Neodymium:Leucine:Urea in the molar ratio
1:2:1



Absorption Spectra of
Neodymium:Leucine:Thiourea in the
molar ratio 1:2:1



IV. RESULT AND DISCUSSION

Energy Interaction Parameters and Lande's Parameter

Table represents observed and calculated value of energy corresponding to different peaks of Neodymium. The observed energy values can be calculated by using Slater-Condon parameters and Lande's parameter given by equations.

$$E_1 = 14.6818 \times F_2$$

$$E_2 = 0.0768 \times F_4$$

$$E_3 = 1.4844 \times F_2$$

The first column of each table represents positions of energy levels. The second column shows observed energy of each level and the third column represent calculated value of energy. The fourth column represents ΔE . After calculations we got Slater-Condon parameters (F_2, F_4, F_6), Racah parameters (E_1, E_2, E_3), Lande's parameter, Nephelauxetic ratio, R.M.S deviation and bonding parameter. When there is formation of ternary complexes of Neodymium with amino-acids then red shift occurs. On complexation, there is very small change in F parameters and Lande's parameter. After formation of complex these two parameters decrease slightly.

The energy levels of various transitions are experimentally as well as theoretically calculated by using Taylor Series expansion.

$$E_k(F_k, \xi_{4f}) = E_0(F_k^0, \xi_{4f}^0) + \sum \partial E_k / \partial F_k \Delta F_k + \partial E_k / \partial \xi_{4f} \Delta \xi_{4f}$$

$$\text{Where, } k = 2, 4, 6$$

The values of F_2, F_4 and F_6 parameters are computed using Judd-Ofelt relation. Least square fit or partial regression method yields values of ΔF_k and ξ_{4f} . Only f^2 interactions are considered and all spin-orbit interactions are to be neglected. In case of Neodymium Complexes $E_1 > E_3 > E_2$.

Nephelauxetic Ratio, Bonding Parameter and R.M.S Deviation

The bonding in rare-earth complexes is weaker than 3d orbital's. The chemical bond for rare-earth complex is considered to be ionic because of their inert gas electronic configuration. It is due to well shielding of 4f orbitals. But experimentally covalency is observed for some rare-earth complexes. On complexation there is expansion of 4f orbital's which can be expressed in terms of Nephelauxetic Ratio (β).

$$\text{Nephelauxetic Ratio } \beta = F_k^c / F_k^f$$

$$F_k^c$$

Where, c – complex state

f – free ion state

Bonding parameter is

$$b^{1/2} = [(1 - \beta) / 2]^{1/2}$$

$$\delta = (1 - \beta) / \beta$$

For Neodymium - Nephelauxetic Ratio, $\beta > 1$. Therefore, $b^{1/2}$ is not real and $\delta = (1 - \beta) / \beta$ is negative in this present work. Hence all ternary complexes of Neodymium make Ionic bonding with amino-acid and with urea and thiourea

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Solution of Linear programming Problem by Fourier – Motzkin Elimination Technique

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Abstract: A new method has been proposed for solving a Linear Programming Problem (LPP) by adopting "Fourier-Motzkin Elimination Technique". This method is useful than the earlier methods because it takes least time and calculations are also simple. The same has been illustrated by a numerical example.

Key words: Linear Programming Problem, Optimal Solution, Inequalities, Fourier-Motzkin Elimination Technique.

I. INTRODUCTION

Linear Programming is a main branch of Operations Research. Linear Programming Problem is formulated as maximizing/minimizing a linear form of profit/cost function whose variables were restricted to values satisfying a system of linear constraints. Linear Programming is a technique for resource utilization. It indicates how a manager can use his available resources under the given facilities in the most effective way. Linear Programming Problem occurs frequently in production allocation problems in real life situations. Different elimination techniques for solving Linear programming Problems are given earlier by Kannappan et al., Kamarker, Kohler, Sharma et al. and Williams.

In the next section, we describe in brief Fourier-Motzkin elimination technique. Further, Fourier-Motzkin elimination technique is applied on inequalities. In the proposed method, first we convert objective function of Linear programming Problem into an inequality, hence total number of inequalities is the sum of the objective function inequality, constraints inequalities and non-negative constraint inequality. This system of inequalities is solved by Fourier-Motzkin elimination technique. This has been verified by a numerical example.

II. FOURIER –MOTZKIN ELIMINATION TECHNIQUE

For small linear programming problems, the Fourier-Motzkin elimination technique can be used. This method reduces the number of variables in a system of linear inequalities by one in each iteration of the technique.

Equation gives only one solution while inequality gives possibility of many solutions in bounded form, out of which we select maximum or

minimum value according to the problem either we have to maximize or minimize. One can easily verify that max./min. value of linear programming gives max./min. value of objective function of $\sum C_i X_i$ where all C_i are positive.

Here, we have applied Fourier-Motzkin elimination technique for a system of inequalities of the same sign i.e., either less than or equal to (\leq) or greater than or equal to (\geq) in nature. In this technique, there are three classes of inequalities with respect to each variable x_i . The first class consists of inequalities in which the coefficient of x_i is $+1$; the second class consists of inequalities in which the coefficient of x_i is -1 ; and the third class of inequalities are those in which the coefficient of x_i is 0. Here variables are eliminated by combining inequalities in such a way that the variables reduced one by one in every iteration so at last there remains only one variable remains with bounded values. From all the bounded values of last variable, we can find the permissible value of that variable. Finally, we get value of other variables by back substitution of value of the last variable.

III. PROBLEM FORMULATION FOR FOURIER-MOTZKIN ELIMINATION TECHNIQUE

Here we consider the Linear Programming Problem as:

$$\begin{aligned} \text{Max. } Z &= c x \\ \text{s.t. } A x &\leq b \\ \text{and } x &\geq 0. \end{aligned}$$

To apply Fourier-Motzkin elimination technique, we formulate this LPP again by taking objective function as constraints and all constraints of same sign of inequality. Reduced form of LPP for Fourier-Motzkin elimination technique are as:

$$\begin{aligned} \text{Max. } Z & \\ -c x + Z &\leq 0 \\ A x &\leq b \\ -x &\leq 0 \end{aligned}$$

Now variables eliminated by combining the inequalities in such a way that variables reduced one by one in each iteration. If at any stage we get an absurd inequality like $0 \leq d$ where d is a negative number then we conclude that the given LPP has infeasible solution otherwise LPP has feasible solution.

IV. NUMERICAL EXAMPLE

$$\text{Max. } Z = 5x + 3y$$

$$\text{s.t. } 3x + 5y \leq 15$$

$$5x + 2y \leq 10$$

$$\text{and } x, y \geq 0.$$

$$\text{Max. } Z$$

$$-5x - 3y + Z \leq 0$$

$$3x + 5y \leq 15$$

$$5x + 2y \leq 10$$

$$-x \leq 0$$

$$-y \leq 0$$

Or above equations can be written as :

$$-x - \frac{3}{5}y + \frac{1}{5}Z \leq 0$$

(1)

$$x + \frac{5}{2}y \leq 5$$

(2)

$$x + \frac{2}{5}y \leq 2$$

(3)

$$-x \leq 0$$

(4)

$$-y \leq 0$$

(5)

After eliminating x from the inequalities

(5), we have

$$\frac{13}{15}y + \frac{1}{5}Z \leq 5$$

$$- \frac{4}{5}y + \frac{2}{5}Z \leq 2$$

$$13y \leq 15$$

$$13y \leq 2$$

$$-y \leq 0$$

Above equations can be represented as:

$$y + \frac{3}{16}Z \leq \frac{75}{16}$$

(6)

$$-y + Z \leq 10$$

(7)

$$y \leq 3$$

(8)

$$y \leq 5$$

(9)

$$-y \leq 0$$

(10)

After eliminating y from the above inequalities (6) to (10), we have

$$\frac{13}{16}Z \leq \frac{213}{16}$$

$$\frac{2}{16}Z \leq \frac{75}{16}$$

$$Z \leq 13$$

$$Z \leq 15$$

$$0 \leq 3$$

$$0 \leq 5$$

Above inequalities can be written as:

$$Z \leq \frac{213}{16}$$

$$Z \leq 25$$

$$Z \leq 13$$

$$Z \leq 15$$

Out of these values of Z , the only permissible value is $\frac{213}{16}$ that satisfies all the inequalities. On putting the value of Z into the inequalities (6) and (7), we get

$$y \leq \frac{48}{19}$$

$$y \geq \frac{48}{19}$$

Hence, $y = \frac{48}{19}$ is the value that satisfies all the inequalities (6) – (10).

On putting the values of Z and y into (1) – (3), we get

$$x \geq \frac{20}{19}$$

$$x \leq \frac{20}{19}$$

Hence, $x = \frac{20}{19}$ is the value that satisfies all the inequalities (1) – (4).

Optimal solution of given Linear Programming Problem comes out to be

$$x = \frac{20}{19}, y = \frac{48}{19} \text{ and Max. } Z = \frac{213}{19}.$$

V. CONCLUSION

The proposed Fourier-Motzkin elimination technique is quite easy to understand and apply. It takes least computation time as compared to traditional simplex method to solve Linear programming Problems. An illustration is described to simplify the whole procedure and its result can be verified by Graphical method, traditional Simplex method and other existing methods.

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SYNTHESIS, PHYSICAL CHARACTERIZATION AND ANTIBACTERIAL ACTIVITY OF M (III) SCHIFF BASE COMPLEX

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Abstract: The M (III) Schiff base complexes prepared from salicylaldehyde and o-amino benzoic acid. Metal selected for the preparation of complexes was Cr(III), Fe (III) and Mn (III). Hence, there are four metal complexes were synthesized. The chemical structure of the synthesized metal ligand complexes were confirmed IR and NMR spectral analysis. The free Schiff base and its complex have been tested for their antibacterial activity against several pathogenic bacteria, such as *Pseudomonas aeruginosa*, *Proteus vulgaris*, *Proteus mirabilis*, *Klebsiella pneumonia* and *Staphylococcus aureus*. The antibacterial activity was determined by the Agar Ditch technique using DMF (polar) and 1, 4 dioxane (non polar) as solvent. The metal complexes showed differential effect on the bacterial strain. The antibacterial activity is dependent on the molecular structure of the compound, the solvent used and the bacterial strain under consideration. In the non polar solvent 1, 4-dioxane the best antibacterial activity was shown by the Zn complex while in polar solvent DMF, Ni complex of Schiff base showed best antibacterial activity.

Keywords: Schiff base; Antibacterial activity; DMF; 1,4 dioxane; Salicylaldehyde; O-aminobenzoic acid

I. INTRODUCTION

Compound which on dissolution do not give ion of which they are made but instead give complex ion are called co-ordination compounds. Co-ordination compounds exhibit different characteristic properties which depend on the metal ion to which they are bound. The nature of the metal as well as the type of ligand etc. these metal complexes have found extensive application in various fields of human interest. The nature of the co-ordination depends on the metal ion and the donor atoms, as well as on the structure of the ligand and the metal ligand interaction. O-amino benzoic acid and salicylaldehyde compounds are capable to form complex with transition metal ion in the form of Schiff base the complex of Cu (II), Ni (II), Zn (II) and Fe (II) with two Schiff base have been synthesized. Their antibacterial activity towards some clinically important bacteria was evaluated¹⁻³. Some Schiff base complexes derived from salicylaldehyde and histidine with some divalent transition metal ion. In the prepared complexes Cd(II) Schiff base complex showed greater antibacterial activity⁴. Cu(II), Co(II), Ni(II) and Zn(II) metal complexes of new heterocyclic Schiff base derived from 1-amino-5-benzoyl-4-phenyl-1 H-pyrimidine-2-one with salicylaldehyde have been prepared and investigated by elemental analysis, mass, electronic, IR and ¹H NMR spectra.

Octa hedral geometry was suggested for all complexes^{5, 6}. Co (II) and Fe (II) complexes of Schiff base derived from istain with some amino acids were synthesized and identified on the bases of their chemical analysis using IR and electronic spectra. All the complexes were suggested to posses an octahedral geometry⁷. A novel Schiff base ligand derived from 2,2 bis (P-methoxyphenylamine), salicylaldehyde and its transition metal complexes with Mn(II), Co(II) and Cu(II) ion prepared and their spectral properties were investigated⁸. The complex of Cr (II), Fe (III), Co (II) and Ni (II) ion with a Schiff base derived from 1,4-dimethylamino benzaldehyde and primary amines have been prepared and investigated using different chemical techniques, such as elemental analysis, electronic spectra. The obtained chemical analysis data showed the formation of 1:1 (metal:ligand) ratio and the square planar geometry was suggested for Co(II) and Ni(II) complexes and an octahedral for Cr(II) and Fe(II) complexes⁹.

Cu (II) complex of Schiff base have been tested against some pathogenic microorganism, a comparative study of the ligands and complexes indicate that the complexes exhibit higher antibacterial activity than the free ligand and control¹⁰.

Cu(II), Ni(II), Co(II) and Zn(II) complexes as well as ligand were tested for their antibacterial and antifungal properties against some pathogen (*Escherichia coli*, *Staphylococcus aureus*, *Aspergillus niger* and *Fusarium oxysporum*). The antibacterial activity of the Schiff base and its Cr(III) was tested on gram positive and gram negative bacteria, the magnetic moment value of the prepared complex revealed the existence of a diamagnetic character¹¹⁻¹³.

In the present work, complexes of Cr (III), Fe (III), and Mn (III) with Schiff base have been synthesized, characterized the chemical structure by IR and NMR spectral analysis and to study the antibacterial activity of the prepared Schiff base complex derived from salicylaldehyde and o-amino benzoic acid.

II. RESULT AND DISCUSSION

Metal ion plays a vital role in a number of different biological processes through co-enzymatic system. The interaction of these ion with biologically active ligand, for instance in drugs, is subject of great interest. Some biologically active compounds act via chelation, but for most of them little is known about how metal co-ordination influences their activity

The four metal complexes and their respective controls produced different inhibition zones against

the tested bacterial strain. The antibacterial activity of Schiff base metal complexes in DMF (polar) and 1, 4 dioxane (non polar) against *P. aeruginosa* is shown in fig-1. All complexes showed greater activity in the polar solvent DMF, then the non polar solvent 1, 4 dioxane. In DMF, the Ni complexes of Schiff base showed the best activity against *P. aeruginosa*, followed by the Zn complex while in 1, 4 dioxane the best antibacterial activity was showed by the Zn complex, in this study, four metal complexes viz. Cu, Ni, Fe and Zn, were used with Schiff base. The growth of the gram negative bacterium was inhibited by the Ni complex.

The antibacterial activity against the gram negative bacterium *k. pneumoniae* is shown in fig-2. In DMF, the Fe complex showed the greater antibacterial activity, while all the other metal complexes showed negligible activity. In 1, 4-dioxane, only the Fe complex showed antibacterial activity, while all the other complexes showed negligible activity. These results again suggest that the antibacterial activity is affected by the metal and the solvent used for investigation of the antibacterial activity. The antibacterial activity against the gram negative bacterium *P. mirabilis* is shown in Fig-3. The antibacterial activity of metal complexes was greater when DMF was used as a solvent. The best antibacterial activity was shown by the nickel complex in DMF, while in 1, 4 dioxane only Cu and Ni complex showed slight antibacterial activity.

The antibacterial activity of the newly synthesized metal complex against gram negative bacterium *P. valaris* are shown in fig-4. All the metal complexes of the Schiff base in both the solvent showed negligible activity. It was observed that this gram negative bacterium was quite resistant to the synthesized compound. The antibacterial effect of the newly synthesized metal complex on the gram positive bacteria *S. aureus* is shown in fig-5, a different effect of the metal complexes was envisaged against this bacterium strain. In DMF, the Fe complex showed the best antibacterial activity was shown followed by Mn, but in 1, 4 dioxane, the maximum antibacterial activity was shown by Zn complex followed by the Fe complex, but the minimum antibacterial activity was shown by Cu and Ni complex of Schiff base.

It is observed that metal chelates have higher antibacterial activity. This is because of an increase in cell permeability. The lipid membrane which surrounded the cell favors the passage of only lipid soluble materials and it is known that liposolubility is an important factor controlling antimicrobial activity^{14, 15}. In the present study low activity of the some metal complexes may be because of the low lipophilicity of the complexes, because of which penetration of the complex through the lipid membrane was decreased and hence, they could neither block nor inhibit the growth of the microorganisms. This is confirming that antibacterial activity is dependent on the molecular structure of the complex.

III. MATERIAL AND METHOD

Metal salts Cupric chloride, Nickel chloride, Ferrous ammonium sulphate and zinc chloride, Dimethyl formamide (DMF) and 1,4- dioxane were purchased from Sud. Chem. India. Salicylaldehyde and O-aminobenzoic acid were purchased from Fluka. The Antibacterial activity of synthesized Schiff base metal complexes was determined by Agar-ditch method.

IV. EXPERIMENTAL

Preparation of Schiff base

20 Cm³ ethanolic solution of salicylaldehyde (1.22g: 0.01mol) and the same volume of ethanolic solution of O-amino benzoic acid (1.37g: 0.01mol) are mixed. The mixture was stirred for 3-4 hour. This solution was evaporated under vacuum to remove the solvent. The product after filtration washed several time with ethanol and recrystallized from hot ethanol and dried under vacuum the colour of the product is orange and its purity was confirmed by chromatography technique.

Synthesis of the complex

For each metal complex, different metal salt solution were prepared. The compounds used for the synthesis of the Mn, Cr, and Fe complexes were cupric chloride, nickel chloride, ferrous ammonium sulphate and zinc chloride, respectively. A mixture of the Schiff base under investigation (0.01mol, 2.41g) 20Cm³ ethanol and the same amount of the same solvent of M(II) salt (0.01mol, 2.37g) was refluxed for 4-5 hours in a water bath the PH of the solution was maintained by the buffer solution. A colour precipitate was obtained. The precipitate was filtered and washed several time with hot ethanol to remove excess metal ion, respectively. The precipitate was then dried and stored in a desiccator over anhydrous CaCl₂ under vacuum.

Antibacterial activity

Antibacterial activity was determined by Agar-ditch method. The investigated microorganisms were *Pseudomonas aeruginosa*, *Proteus vulgaris*, *Proteus microbiles*, *Klebsiella pneumoniae* and *Staphylococcus aureus*. The metal complexes were dissolved in one of the two solvent 1, 4 dioxane (non polar) or DMF (polar) solvents to obtained final concentration 1mg/0.1ml. A loop full of the given test strain was inoculated in 30ml of nutrient broth and incubated for 24 hour in an incubator at 30°C in order to activate the bacterial strain activity. 18-20 ml of the nutrient agar media was added in to a 100mm diameter pantry-plate. 0.1ml of the activated strain was inoculated in to the media when it reaches the temperature of 40°C. The medium was allowed to solidify. After solidification of the media a hole was made in the plates with the help of a cup-borer, which was then filled with one of the test sample solution. Controls were run (for each bacterial strain and each solvent), where pure solvent was inoculated in to the hole. The plates were incubated for 24 hours at 35°C. The inhibition zone formed by these compounds against the particular test bacterial strain determined the antibacterial activity of the synthetic complexes. The mean value obtained for three individual

replicates was used to calculate the zone of growth inhibition of each sample.

CONCLUSION

For the above results, it can be concluded that amongst the four metals used for complexes formation, in non polar solvent 1, 4 dioxane Zn complex of Schiff base showed the best antibacterial activity but in polar solvent DMF, Ni complex showed best antibacterial activity followed by Zn and Fe complex. Cu complex showed negligible antibacterial activity.

Acknowledgement:

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Table 1. The structure of the metal complexes was confirmed by I.R (KBr, cm^{-1}) analysis.

| Complex | -OH (Stretching) | -OH (Bending) | -C=N (Stretching) | M-N | M-O |
|----------------------------|---------------------|------------------|----------------------|-----|-----|
| Cu(II) Schiff base Complex | 3341 | 1350 | 1511 | 744 | 530 |
| Ni(II) Schiff base Complex | 3306 | 1354 | 1539 | 750 | 497 |
| Fe(II) Schiff base Complex | 3136 | 1332 | 1565 | 685 | 475 |

Table 2. Analytical data (CHN) of divalent Cu, Ni, Fe and Zn Schiff base complexes.

| Complex | M | C | H | N | Colour | Mr g mol ⁻¹ |
|-----------------------------|------------------|------------------|----------------|----------------|------------------|------------------------|
| Mn(III) Schiff bas Complex | 19.80 (19.81) | 52.29 (52.41) | 3.35 (3.43) | 4.31 (4.36) | Dark brown | 315 |
| Cr(III) Schiff base Complex | 18.50 (18.59) | 53.18 (53.21) | 3.46 (3.48) | 4.42 (4.43) | Yellowish orange | 316 |
| Fe(III) Schiff base Complex | 17.78 (17.84) | 53.65 (53.70) | 3.48 (3.51) | 4.36 (4.47) | Yellowish brown | 313 |

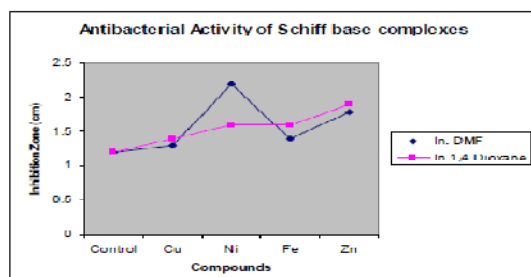


Fig-1. Antibacterial activity of Metal Schiff base complexes in DMF and 1,4-dioxane against *P. aeruginosa*

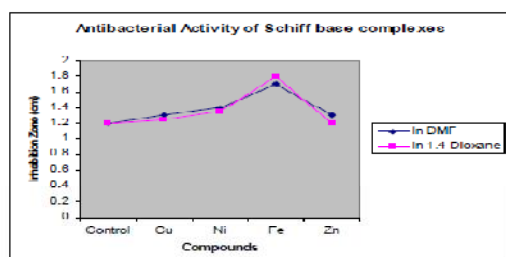


Fig-2. Antibacterial activity of Metal Schiff base complexes in DMF and 1,4-dioxane against *K. pneumoniae*

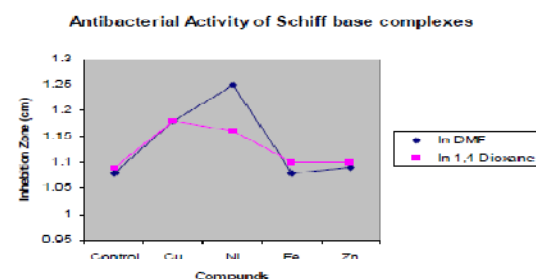


Fig-3. Antibacterial activity of Metal Schiff base complexes in DMF and 1,4-dioxane against *P. mirabilis*

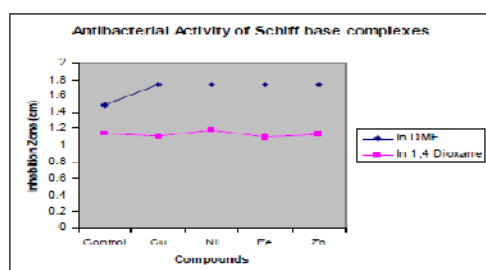


Fig-4. Antibacterial activity of Metal Schiff base complexes in DMF and 1,4-dioxane against *P. valaris*

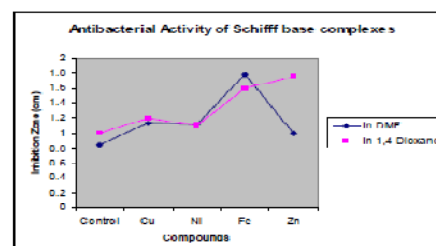
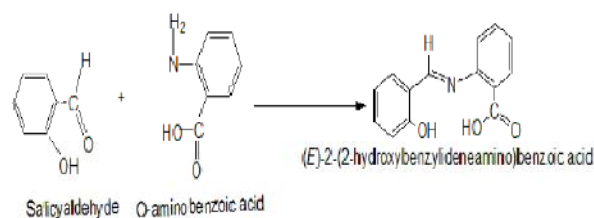
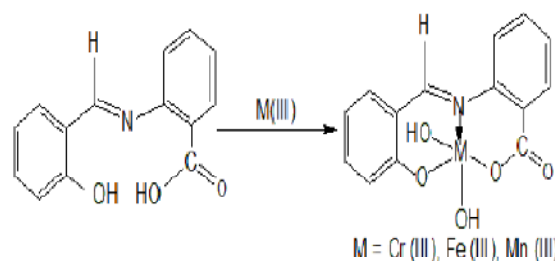


Fig-5. Antibacterial activity of Metal Schiff base complexes in DMF and 1,4-dioxane against *S. aureus*



Scheme I



Schiff base metal complex

Scheme II

FPGA Implementation and Optimization of Highly Linear Wideband Chirp Generation for FMCW Radar Application using Fractional-N PLL

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Abstract This work addresses the FPGA implementation and optimization of Fractional-N Phase Locked Loops (Frac-N PLLs) used to generate frequency chirps for Frequency Modulated Continuous Wave (FMCW) radar applications. In a Fractional-N PLL, we have two main clock domains which are the reference and the divided VCO clock domains. Clock domain crossings need to be considered during chirp generation to produce linear chirps. In addition, increases in the integer divide ratio during the generation of chirp can cause transient frequency glitches that also affect the chirp linearity if they are not taken care of. In this work we propose implementation techniques to address these issues in Fractional-N PLLs. The proposed techniques can be used for linear wideband chirp generation and It also improve the distance accuracy by a factor of 1.5 and the distance precision by a factor of 1.0.

Keywords— Phase Locked Loops, Radar, Chirp, Multi Modulus Divider (MMD), Sigma Delta Modulator (SDM), Frequency Modulated Continuous Wave (FMCW)

I. INTRODUCTION

In recent past years due to their compact design Fractional-N PLL have been used in the application of frequency modulation and reference frequency generation. Due to high reference frequency used in PLL, it achieves fine frequency step by the Multi Modulus Divider (MMD) integer division ratio dithering, using a Sigma Delta Modulator (SDM). So that on average, a fractional division ratio generated

In the application of FMCW radar, Fractional-N PLL is used for frequency chirp's generation. This is the basic signal used for distance calculation in this type of applications. For chirp generation, Fractional-N PLL integer and fractional division ratio is incremented regularly by very small steps with the rate faster than PLL loop bandwidth, so that smooth frequency ramp which represents desired linear chirp is generated at the PLL output.

Generated chirp is then transmitted, which travel at the speed of light and lastly mixed with locally generated chirp at the receiver, which is synchronized with transmitted chirp.

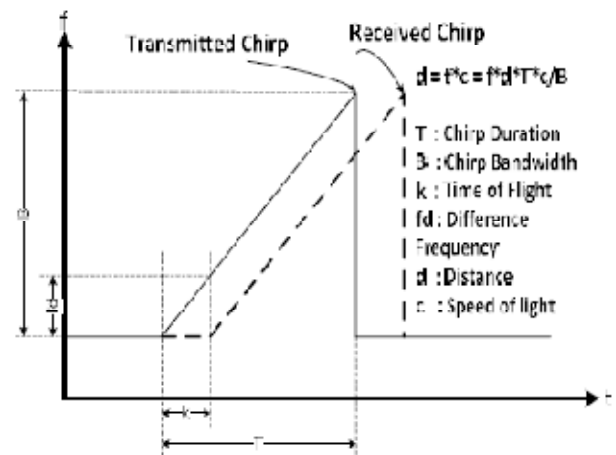


Figure 1. FMCW Radar Principal

The outcome is baseband single tone with frequency directly proportional to the time of flight (distance) between the receiver and transmitter as shown in Figure 1. Assuming that chirp is entirely linear which indicate constant gradient.

Consideration of many aspect need to be taken care, while optimizing a Fractional-N PLL for application of radar. This is because of requirement of wide chirp bandwidth for achieving exceptional range resolution [1, 4, 5, 7].

In [3] introduced a Fractional-N PLL that integrate a wideband Voltage Controlled Oscillator (VCO) which optimized for FMCW radar applications by specially incorporating a single wide tuning range.

As indicated that generated chirp should be extremely linear, mean having low RMS (root mean square) error. In Fractional-N PLL the sigma delta modulator (SDM) used divided VCO clock while the counter for chirp generation used for incrementing the division ratio is clock by the reference clock. Due to this, for generation of extremely linear

This paper is organized as follows: In section II, discussed the clock domain crossing issue in detail and recommend a solution for it. In section III, Integer division glitch issue is discussed and recommend a solution. In section IV, Simulation results shown for validating the result to make evident for the proposed concepts and methods. In section V, the results from this work is concluded.

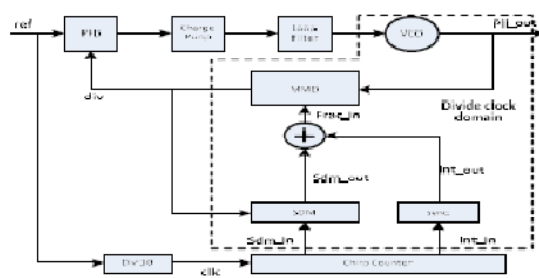


Figure 5. Proposed Frac-N PLL with clock domain crossing

periods is depend on the signal delta modulator (SDM) order and the number of the output quantization levels. In general, the variation of the edges is much smaller than the reference clock period. In case of the FMCW radar Fractional-N PLL, generally the 3rd order sigma delta modulator (SDM) is used with the output quantization level from +4 to -3. So when the PLL is locked the positive edge of div clock is within -1.8 to +2.3 VCO period range from the positive edge of the reference clock as per out simulation. In case of integer-N PLL during the lock condition, the feedback loop forces the positive edge of the reference clock and div clock will be exactly aligned.

Although this fact may seem to add more difficulty to the problem because it adds more uncertainty during bus synchronization like that due to meta-stability, but we can still use it to our benefit as follows.

For FMCW radar application we can conclude that for any PLL at lock condition the negative edge of the reference clock is always away from the positive edge of the div clock and is approximately in the middle of the div period assuming a 50% duty cycle reference clock and so we can treat both the reference and div clock is synchronous to each other and belong to same clock domain if launching data at negative edge and capturing it on positive edge.

So, we can simply use the negative edge of the reference clock to generate `int_in` and `sdm_in` and use the positive edge of the `div` clock to capture the data in sigma delta modulator (SDM). By using this we can avoid the synchronizer which in turn achieve the power, area and complexity optimization as shown in Figure 4. One register is added to integer part for align the fractional and integer data in `div` clock domain.

Figure 5 shows the timing diagram with the proposed solution. We can see that the uncertainty in the timing of the new captured data is reduced in our case to approximately 2 VCO periods which is much less than the original uncertainty of 1 div period. The improvement can be approximated to be equal to $N_{div}/2$ where N_{div} is the nominal integer divide ratio.

For example, in our FMCW system F_{ref} is 15 MHz and F_{vco} is 2.43 GHz so N_{div} is 162. Then the uncertainty due to clock domain crossing is 81 times less in our proposed scheme.

Note that this solution was possible in the specific case of PLLs under lock condition because the div clock can be considered as a derived clock from the ref clock i.e. they are

not strictly of different origins. But for other general cases of arbitrary clock domain crossing a bus synchronizer is a good option.

IV. INTEGER DIVISION GLITCH ISSUES

A. Problem Definition

Integer division glitch issue needs to be carefully addressed while designing Fractional-N PLLs for FMCW radar

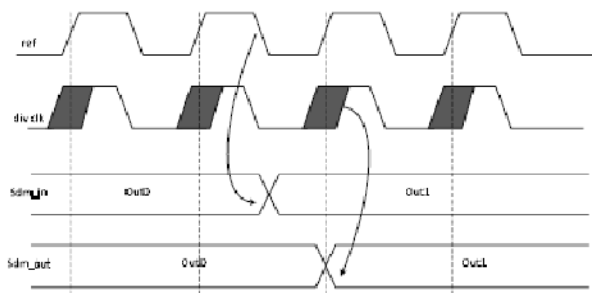


Figure 4. Timing Diagram for Proposed synchronization method

applications. Most of the case where the chirp bandwidth is larger than the reference frequency, it shows that during the chirp generation, when the fractional part is increased gradually and reaches its full scale then and it needs to roll over. During the rollover integer path also needs to be incremented by 1. So, a glitch in the output frequency might occur as shown in Figure 6.

This indicates that the response for incrementing `int_in` is faster than that for rolling over `sdm_in` since the output frequency first increases rapidly then decreases again before it resumes the normal chirp gradient. The root cause of this issue is that the SDM includes some delay from its `sdm_in` to its `sdm_out` that is larger than the delay from `int_in` to `int_out`. So that the larger delay difference causes the larger the magnitude of the glitch.

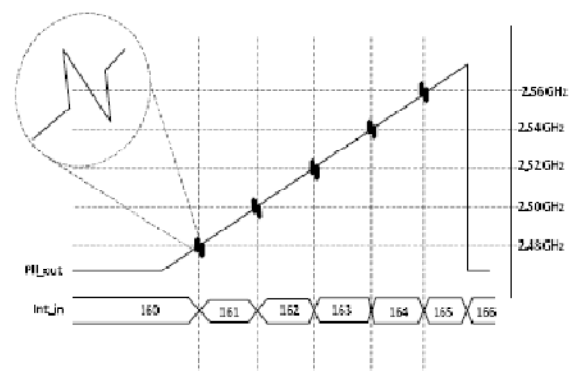


Figure 6. Frequency Chirp Containing Integer division glitches

The magnitude of this frequency glitch is almost unnoticeable compared to the carrier frequency. And again, in most applications this is only a transient effect that most of the time has no impact on the system performance.

For an FMCW radar system, due to down converting the chirp to the baseband at the receiver, the glitches are in few MHz range which is largely comparable to the baseband frequency. This is required to affect the calculation of beat frequency by the Fast Fourier Transform (FFT) algorithm in the FPGA even more than the clock domain crossing issue as the errors due to this effect on the baseband signal may be in the order of few MHz while the errors due to the clock domain crossing issue are in the order of few KHz. The impact of these glitches on the distance calculation accuracy and precision will be also shown in section IV.

B. Proposed Solution to the Integer Division Glitch Issue

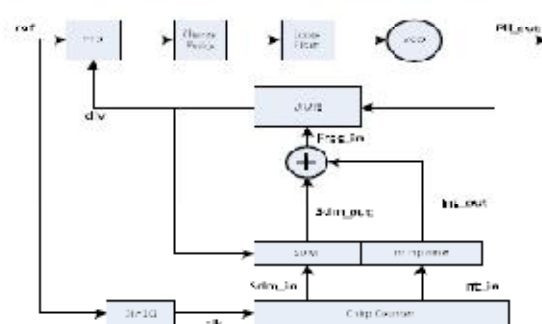


Figure 7. Proposed Block Diagram of Frac N PLL for FMCW Radar

To solve this issue, we propose introducing several pipelining stages in the path of int_in to balance the delay introduced by the sigma delta modulator (SDM) from sdm_in to sdm_out as shown in Figure 7. This way, the integer and fractional parts of the division word now occur at the MMD together rather than consecutively and so we can now guarantee highly linear frequency chirps.

The SDM is based on a MASH 1-1-1 architecture. Doing the Z-domain analysis we found that it has a signal transfer function of Z^{-4} from sdm_in to sdm_out . Therefore, 4 pipelining stages are used to delay int_in by the same 4 div clock cycles. This way we could get a highly linear wideband chirp as shown in Figure 8.

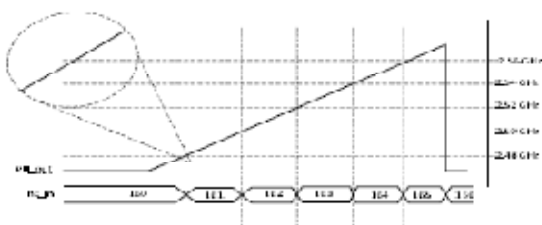


Figure 8. Chirp using optimized Frac-N PLL

V. SIMULATION RESULTS

For verification of the above concepts and methods, we built a simulation environment where we can run the digital chirp counter and SDM with models for the PLL building blocks. This way we can simulate the complete chirp transmission and mixing at the receiver and resulting baseband is recorded vs time in a file. This data is again processed using MATLAB to calculate the distance by doing FFT transformation after that peak detection. The first general observation is that the resulting baseband spectrum is significantly cleaner after optimization as shown in Figure 9. After the we performed multiple simulations.

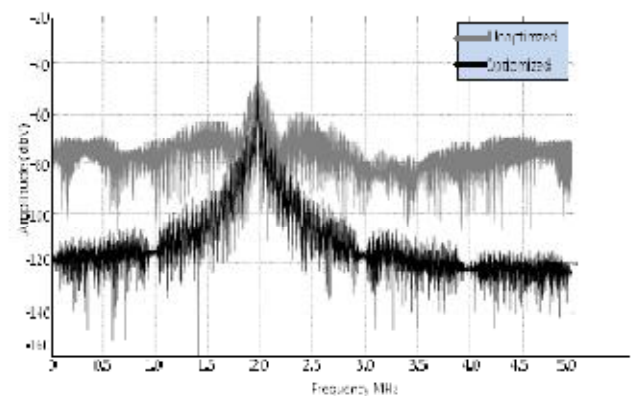


Figure 9. FFT of baseband before and after optimization

A. Accuracy Simulation

The first few set calculates the distance error for 13 equally spaced distances. This gives an indication about the system's accuracy. We can see from the results Figure 10 in that with the proposed techniques, accuracy was improved by more than a factor of 1.5. Another improvement is that the accuracy is almost constant vs distance. We can observe that the integer division glitch has a stronger effect on the accuracy than the clock domain crossing issue as expected.

B. Precision Simulation

The second simulation set calculates the distance error in 10 consecutive chirps but this time for the same distance. This gives an indication about the system's precision. We can see from the results in Figure 11 that with the proposed techniques, precision was improved by around a factor of 1.5.

We can again observe that the integer division glitch has a stronger effect on the precision than the clock domain crossing issue.

It is worth mentioning that we expect better results in measurements since our simulation setup has some limitations on the timing accuracy. Namely, it is difficult for the simulator To resolve a frequency difference of 1 Hz (which indicate to a distance of 5 mm) from the 2.8 GHz carrier without some numerical error. That is why in our simulations the precision of the optimized systems seems to be closed to that of the one with the clock domain crossing issue.

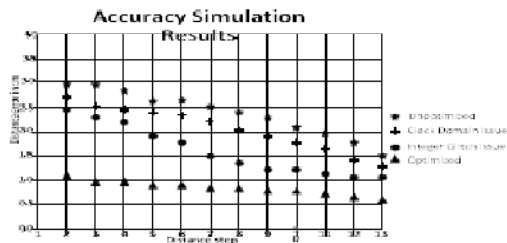


Figure 11. Accuracy Simulation Results

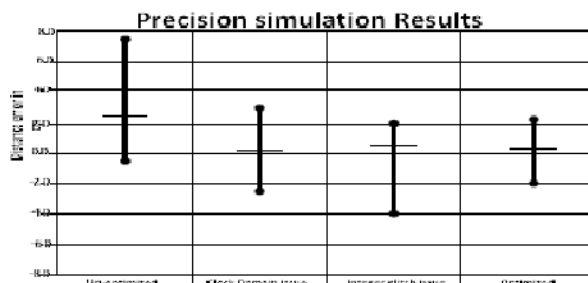


Figure 10. Precision Simulation Results

Table 1 compares our system to some works on FMCW radars. Note that in [3] and [4] a prescaler is used before the MMD, so we normalized the chirp bandwidth by the prescaler divide ratio. Also, for fair comparison we refer the frequency resolution and RMS frequency error to the VCO even if it is followed by a frequency multiplier as in [5]. We can see that we have the least RMS error while having the widest chirp bandwidth relative to the reference frequency.

TABLE I. COMPARISON OF PROPOSED SYSTEM TO STATE OF THE ART

| | [3] | [4] | [5] | This Work | Unit |
|------------------------|-----|------|------|-----------|------|
| VCO Center Freq | 77 | 77 | 4.25 | 2.43 | GHz |
| Chirp bandwidth at MMD | 175 | 8.75 | 500 | 120 | MHz |
| Reference freq | 700 | 50 | 160 | 15 | MHz |
| Freq resolution at VCO | 43K | 3 | N/A | 0.8 | Hz |
| RMS freq error at VCO | 60 | 50 | 19 | <8 | KHz |

VI. CONCLUSION

This paper presented optimization techniques for Frac-N PLLs used for highly linear wideband chirp generation for FMCW radar applications. A synchronization scheme was proposed to address clock domain crossing issues. Moreover, an equalization scheme was proposed to mitigate integer division glitch issues thus improving the distance calculation accuracy by a factor of 2 and precision by a factor of 1.5.

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