MATERIALS AND METHODS

CHAPTER - III
MATERIALS AND METHODS

In any research work the materials and the methods adopted are the aspects, which decide and determine qualitatively and quantitatively the outcome of the research. The design of the present investigation on the thesis entitled "Inhibitive Action of *Cocos nucifera* L. (Coconut palm) and *Borassus flabellifer* L. (Palmyra palm) – Shell, Leaf Stalk and Peduncle Extracts on the Corrosion of Mild Steel in Acidic Media and their Adsorption Characteristics" consisted of the following steps.

- ✶ Selection of metal, inhibitors and acid medium.
- ✶ Characterization of inhibitors using FT-IR and GC-MS techniques.
- ✶ Corrosion inhibition studies using mass loss method and electrochemical impedance spectroscopy.
- ✶ Surface Analytical Techniques.
- ✶ Quantum chemical study.

3.1 SELECTION OF METAL, INHIBITORS AND ACID MEDIUM

In the current investigation, the aqueous extract from destructive distillation method of shell, leaf stalk and peduncle of coconut palm and palmyra palm were selected as inhibitors on mild steel corrosion in 1 M HCl and 0.5 M H_2SO_4.

3.1.1 Selection of the Sample

Mild steel sample has been selected for the present study. It was selected due to its wide application in industries, easy availability and being less expensive. Since it suffers from severe corrosion in aggressive environment, it has to be protected. In fact, mild steel is the most widely used engineering material, accounts for approximately 85%, of the annual steel production worldwide. Despite its relatively limited corrosion resistance, carbon steel is used in large tonnages in marine applications, nuclear power and fossil fuel power plants, transportation, chemical processing, petroleum production, pipelines, mining, construction and metal-processing equipment. Because carbon steels represent the largest single class of alloys in use, both in terms of tonnage and total cost, it is easy to understand that the corrosion of carbon steels is a problem of enormous practical importance. These facts call for a research to use mild steel for the entire study.

3.1.2 Preparation of the Sample

Rectangular specimens of working surface area 5x1cm^2 were used for mass loss measurements and 1x1cm^2 with 5 cm long stem (isolated with Teflon tape) for the electrochemical methods. The specimens were polished mechanically using emery papers and worked thoroughly with triple distilled water, degreased with acetone and dried using air flow at room temperature and kept in a moisture free desiccator for further studies. The mild steel specimens used had the following percentage elements of composition as shown in Figure - 12.

Figure - 12 Chemical composition of mild steel specimen

3.1.3 Selection of Medium

Due to tremendous increase in industrial activities, H_2SO_4 and HCl is a vital commodity in the world. It is widely used for de-rusting, pickling, cleaning of refinery equipment and removal of calciferous deposits from boilers, radiators of vehicles, pipeline carrying water or petroleum products, heat exchangers etc. Hence 0.5 M H_2SO_4 and 1 M HCl were selected to study the inhibitive effect of aqueous extract from destructive distillation of shell, leaf stalk and peduncle of coconut palm and palmyra palm on corrosion of mild steel. 0.5 M H_2SO_4 and 1 M HCl solutions were prepared from analytical grade reagents and de-ionized water was used for preparing the solution.

3.1.4 Selection of the Inhibitor

The use of inhibitor in corrosion prevention has been well established and numerous inhibitors have been documented. It is revealed that there are some inhibitor compounds in plants that can inhibit corrosion in acidic environment. The choice of the present inhibitor is based on the following considerations.

- Easy availability.
- Biodegradable.
- Non toxic.
- Environmentally acceptable.
- Non-hazardous.
- A renewable source.

Plant extracts are incredibly rich sources of naturally synthesized chemical compounds (eg., amino and organic acids, glucosinolates, alkaloids, polyphenols, tannins) and most are known to have inhibitive action. For the present study, aqueous extract from destructive distillation of shell, leaf stalk and peduncle of *Cocos nucifera* L. (Coconut palm) and *Borassus flabellifer* L. (Palmyra palm) were used as corrosion inhibitor for mild steel (MS) in 0.5 M H_2SO_4 and 1 M HCl (Figure-13).

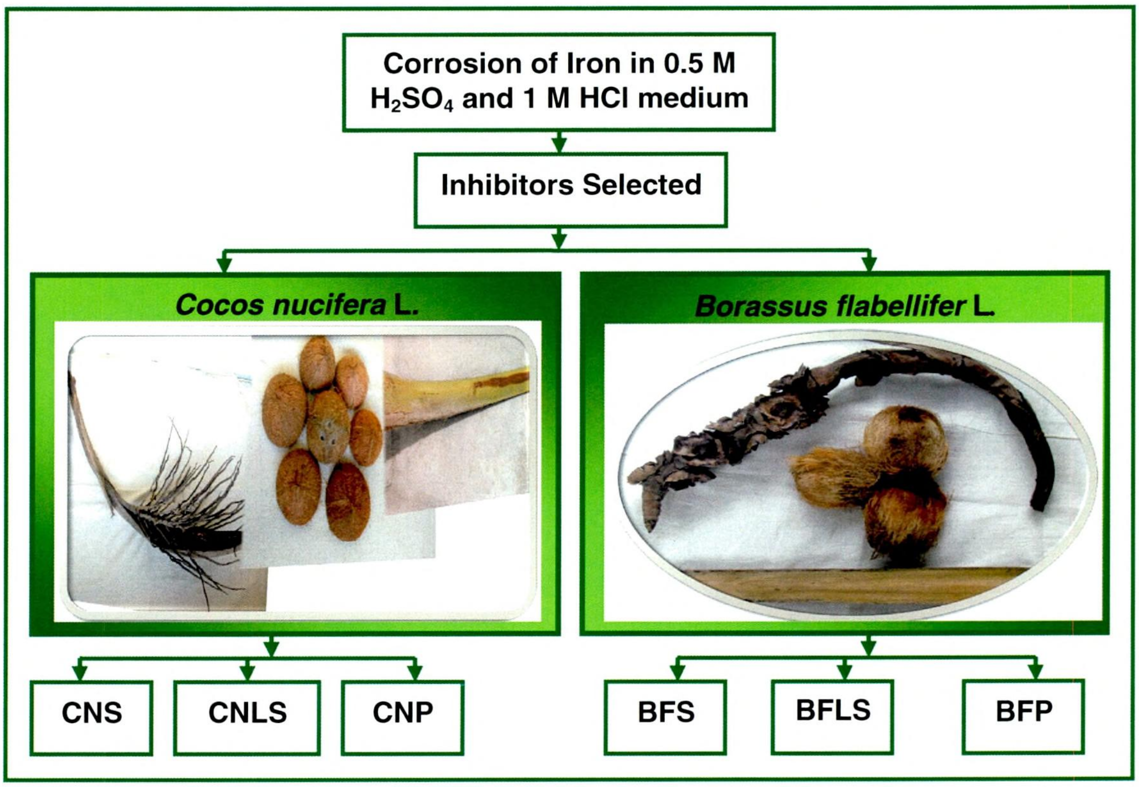


Figure - 13 The selected inhibitor system

3.1.5 Preparation of Inhibitors by destructive distillation

The inhibitor used for this study was the shell, leaf stalk and peduncle of coconut palm and palmyra palm. Plant materials have been carried out by several researches **(Demirbas, 2004; Caglar and Demirbas, 2000)** based on this standard procedure that plant materials such as CNS, CNLS, CNP, BFS, BFLS and BFP were collected, at Sirumugai of Coimbatore district in Tamil Nadu, India and destructive distillation process was carried out. Destructive distillation may be described as the thermal degradation of materials in the complete absence of inadequate presence of oxygen **(Bridgwater and Bridge, 1991)**. Three products are usually obtained from destructive distillation process: gas, liquid and char. Destructive distillation is being considered to be an emerging, new and potential technology to produce value-added products, fuels and chemicals from oil palm waste.

In the present work the inhibitors are obtained by destructive distillation from two popular species: *Cocos nucifera* L. (Coconut palm) and *Borassus flabellifer* L. (Palmyra palm). Palm waste such as shell, leaf stalk and peduncle were cleaned, chopped into small pieces, air dried and stored at room temperature prior to use. 250 gm of air dried pieces was transferred to a 2000 ml round bottomed flask, directly heated in a mantle with water condenser at about 80˚C in the absence of air and without a carrier solvent (destructive distillation) (Figure - 14).

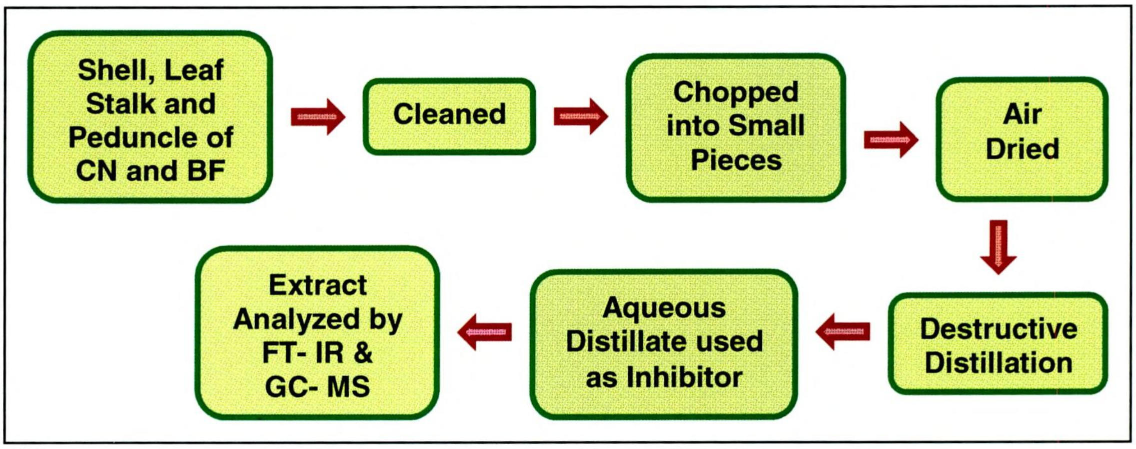


Figure - 14 Preparation of CN and BF extracts

The products obtained are i) A gaseous mixture or wood gas. ii) **aqueous distillate obtained which was used as inhibitor.** iii) a thick black liquid or wood tar which was separated from the aqueous distillate using a separating funnel. iv) solid residue or wood charcoal was left in the round bottomed flask. It is popularly a domestic fuel. The aqueous extracts obtained from respective sources were entered in the Table - 1.

Table – 1 Amount of aqueous extract obtained using 250 g of CN and BF

Code	Plant	Popular name	Plant part	Aqueous extract (mL / 250 g)	Type of extraction
CNS	*Cocos nucifera* L.	Coconut palm	Shell	120	Destructive distillation
CNLS			Leaf stalk	85	
CNP			Peduncle	100	
BFS	*Borassus flabellifer* L.	Palmyra palm	Shell	95	
BFLS			Leaf stalk	80	
BFP			Peduncle	90	

3.2 CHARACTERIZATION OF CN AND BF EXTRACTS

Characterization of CN and BF extracts were effectively done by using FT-IR studies and GC-MS analysis.

3.2.1 FT-IR

FT-IR spectroscopy is an excellent technique for the qualitative analysis, the spectrum of compound is unique. Information about the structure of a molecule could frequently be obtained from its absorption spectrum. To find out the functional groups present in the aqueous extracts FT-IR study has been conducted. The sample for FT-IR studies were prepared by finely mixing the extract with spectroscopically pure KBr and then pressed by using a die so as to get a fine transparent pellet. The FT-IR spectrum was recorded for shell, leaf stalk and peduncle of CN and BF extracts with a frequency ranging from 4000 to 400 cm^{-1} using BRUKER Optik GmbH FT-IR spectrometer MODEL No – TENSOR 27 with the SOFTWARE – OPUS version 6.5 (CECRI – India).

3.2.2 GC- MS Analysis

Gas Chromatography (GC) and Mass Spectrometry (MS) make an effective combination for chemical analysis. GC analysis separates all the components in a sample and provides a representative spectral output. Following the injection of the sample into the injection port of the GC instrument the sample vaporizes, separates and analyzes the various different components. Each component ideally produces a specific spectral peak that may be recorded on a paper chart or electronically. The time elapsed between injection and elution is called the "retention time". The retention time can help to differentiate various compounds. The size of the peaks is proportional to the quantity of the corresponding substances in the specimen analyzed. The peak is measured from the baseline to the tip of the peak. The GC-MS analysis with the chromatogram and m/z spectrum, were analyzed with the hit compounds by comparing with the inbuilt library, with the help of NIST'08 software. To identify the probable constituents responsible for the inhibition, the chemical composition of the shell, leaf stalk and peduncle of CN and BF extracts were studied by use of gas chromatography and mass spectrometry (GC-MS).

In order to identify the individual compounds in the aqueous distillate of CNS, CNLS, CNP, BFS, BFLS and BFP extracts gas chromatograph-mass spectrometry (GC-MS) technique was used **(Kawser and Farid Nash, 2000; Goh Meng Seng, 2006)**. The GC-MS instrument was Fisons 800 Top GC coupled to Fisons MD 800 series MS quadrupole mass detector. The aqueous distillate was desorbed in GC injector at 100°C for 2 minutes in splitless mode and chromatographic separation was carried out on a 30 m x 0.25 mm x 0.25 µm film thickness DB-5MS (5 % phenyl - 95 % methyl polysiloxane) capillary column. The GC oven temperature was programmed from 100°C (held for 1 min.) to 250°C at a rate of 6°C. Helium was used as a carrier gas at a constant flow of 1.0 mL/min. Mass spectra was recorded in electron impact mode at 70 eV, scanning the 20 - 550 m/z range. The interface and source temperature were 200°C and 250°C, respectively.

The identification of the isolated volatile compounds was achieved by comparing obtained mass spectra of unknown peaks with those stored in the NIST (National Institute of Standards and Technology) and Wiley mass spectral electronic libraries. Identifications were confirmed by comparison with authentic substances used as references and by use of linear retention indices (LRI). Relative area values (as a percentage of total volatile composition) were directly obtained from total ion current (TIC). All analyses were carried out in duplicate (SITRA-India).

3.3 TECHNIQUES ADOPTED

The use of inhibitors is the most economical and practical method in reducing corrosive attack on metals.

3.3.1 Mass Loss Methods

3.3.2 Electrochemical Methods

- ✶ Potentiometric Polarisation Method.
- ✶ Linear Polarisation Resistance Method.
- ✶ Electrochemical Impedance Spectroscopic Techniques

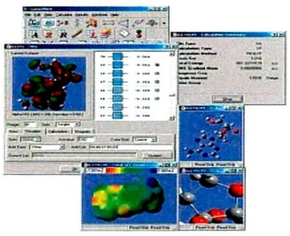
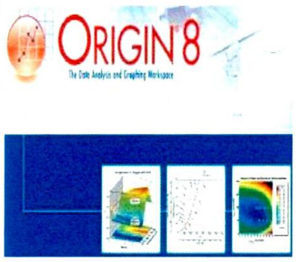
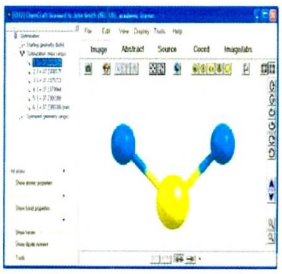
3.3.3 Surface Analytical Techniques

- ✶ Fourier Transform Infrared Spectroscopy (FT-IR).
- ✶ Scanning Electron Microscope (SEM).

3.3.4 Molecular Modeling/ Quantum Chemical approach/ Computational details

3.3.5 Software Tools

Table - 2 List of software Tools

Software	Name of the software	Software	Name of the software
	Gaussian 03		Origin 8
	Chemcraft 1.6		SPSS 12

3.3.1 Mass Loss Method

It is one of the oldest techniques of monitoring corrosion and is based on exposing the coupons of the metal on to the test media for a predetermined period of time, then removed, washed kept in the desiccators and then the mass loss of coupons are measured. Mass loss measurements were performed with dried rectangular strips following ASTM standard procedure **(stated in ASTM, G 1-2, and 1996a).**

In the present work, weighed test pieces were immersed in triplicate in the test media (100 mL) viz., 0.5 M H_2SO_4 and 1M HCl with varying concentrations of the inhibitor. They were removed after a particular period of immersion, washed dried and reweighed. The experiments were performed for various parameters such as,

* Concentration variation from 0.5%v/v to 4.0%v/v
* Different time intervals: 1/2 h, 1 h, 3 h, 6 h, 12 h, 24 h.
* Various temperatures: 313 K, 323 K, 333 K, 343 K.

(For temperature study the time of immersion was 1/2 an hour). The specimens were abraded with abrasive papers 320, 400 and 600 grit, washed in absolute ethanol and acetone, dried in room temperature and stored in the moisture free desiccators before their use in corrosion studies. The specimens are weighed before immersion in the test solutions and reweighed after immersion. From the initial and final masses of the specimen, the mass loss was calculated. From the mass loss - Corrosion rate, Inhibition Efficiency and surface coverage were determined using the following relationship.

The expressed as mills per year was calculated using the formula,

$$\text{Corrosion Rate (mpy)} = \frac{534xW}{DAT} \text{ x } 100 \qquad (3.1)$$

where, W = Weight loss in milligram; D = Density of mild steel in g / cm^3; A = Area of the specimen in cm^2; T = Exposure time in hours

$$\text{Inhibitor Efficiency (\%)} = \frac{CR_{blank} - CR_{inh}}{CR_{blank}} \text{ x } 100 \qquad (3.2)$$

where, CR_{blank} = CR of MS in acidic medium (0.5 M H_2SO_4 and 1 M HCl, respectively); CR_{inh} = CR of MS in the presence of inhibitor (Shell, Leaf Stalk and Peduncle of CN and BF, respectively) and acidic medium (0.5 M H_2SO_4 and 1 M HCl, respectively).

$$\text{Surface Coverage } (\theta) = \frac{W_o - W}{W_o} \qquad (3.3)$$

where, W_o = Weight loss of MS without inhibitor (blank); W = Weight loss of MS in the presence of the inhibitor.

Adsorption Isotherm

It is generally accepted that organic molecules inhibit corrosion by adsorption at metal/solution interface and that the degree of adsorption depends on structure of the molecules, the chemical composition of the solution, the nature of the metal surface, the temperature and the electrochemical potential at the metal/solution interface **(Rigg, 1967)**. Adsorption provides information about the interaction among the adsorption molecules themselves as well as their interaction with the electrode surface. A useful method that assists in the understanding of the mechanism of organo electrochemical reactions in the adsorption process is the adsorption isotherm **(Singh and Quraishi, 2010)**. An adsorption isotherm gives the relation between the coverage of an interface with the adsorbed species (the around adsorbed and the concentration of species and the solution).

In acid corrosion, generally it is assumed that inhibitors act through a process of adsorption on the metal surface. The adsorption of inhibitor may determine the structural change of the double layer thus reducing the rate of electrochemical partial reaction. The knowledge of the adsorption behaviour of the inhibitor is therefore important for the defined of its active mechanism. For this reason, the dependence of surface coverage on concentration is studied through the following adsorption isotherm.

Langmuir	⟶	log (C/θ) Vs log C	(3.4)
El – Awady	⟶	log (θ/1- θ) Vs log C	(3.5)
Temkin	⟶	θ Vs log C	(3.6)
Freundlich	⟶	log θ Vs log C	(3.7)
Frumkin	⟶	θ Vs ln [θ / C (1- θ)]	(3.8)
Flory – Huggins	⟶	log (θ/C) Vs log (1- θ)	(3.9)

Various adsorption isotherms are tested graphically to fit a suitable adsorption model for the inhibitor. Data were tested graphically by fitting various isotherms and statistical estimation of correlation for the curve fitting of isotherms have been used to investigate the goodness of fit of the isotherms using SPSS 12 package. A straight line will indicate that the inhibitor adsorbed through adsorption isotherms whereas 'S' shaped curve in the case of Frumkin indicate the inhibitor adsorbed through Frumkin isotherm.

Energy of Activation (E_a)

The activation energy for the corrosion of mild steel in 0.5 M H_2SO_4 and 1M HCl was calculated using the Arrhenius equation **(Radovici, 1965).**

$$CR = A \exp(-E_a / RT) \qquad (3.10)$$

Where CR is the corrosion rate of mild steel, A is Arrhenius or pre-exponential constant, E_a is the activation energy for the corrosion of mild steel, R is the gas constant and T is the temperature. The logarithm of both sides of equation (3.10) yields equation (3.11)

$$\log CR = \log A - E_a/2.303RT \qquad (3.11)$$

Applying the formula $Ea = - 2.303 \times R \times Slope$

Plots of log CR Versus 1/T for the corrosion of mild steel in the presence of various concentrations of CN and BF extracts yields straight lines. From slopes and intercepts of the Arrhenius plot, the values of E_a and A were computed.

The transition state equation (3.12) was used to calculate some thermodynamic parameters (enthalpy of adsorption ΔH_a and entropy of adsorption ΔS_a) for the adsorption of CN and BF extracts on mild steel surface.

$$CR/T = R/Nh \times \exp(\Delta S_a/R) \times \exp(\Delta H_a/RT) \qquad (3.12)$$

Where CR is the corrosion rate, R is the universal gas constant (8.31434 $JK^{-1}mol^{-1}$), T is the absolute temperature, A is the pre-exponential factor, h is Planck's constant (6.626176×10^{-34} JS) and N is Avogadro's number (6.02252×10^{23} mol^{-1}).

From the logarithm of both sides of equation (3.12), equation (3.13) is obtained

$$\log (CR/T) = \log R/Nh + \Delta S_a/2.303R - \Delta H_a/2.303RT \qquad (3.13)$$

Plots of log (CR/T) versus 1/T for CN and BF extracts were linear. The slopes and intercepts of the transition state plots, the values of ΔS_a and ΔH_a are calculated.

Thermodynamic Parameters

Free Energy of Adsorption (ΔG°_{ads})

The change in free energy of adsorption at high temperature at various concentrations has been calculated using the formula, **(Umoren *et al.,* 2007a)**.

$$\log C = [\log (\theta/1-\theta)] - \log B \qquad (3.14)$$

Where $\log B = -1.744 - \Delta G_{ads}/2.303\ RT$

$$-\Delta G^o_{ads} = 2.303\ RT\ (1.744 + \log (\theta/1-\theta) - \log C) \qquad (3.15)$$

where, R = Gas constant (8.314 J/mole); T = Temperature in Kelvin;

C = Concentration (%v/v); θ = Surface coverage.

Enthalpy (ΔH°_{ads}) and Entropy (ΔS°_{ads}) of Adsorption

According to Gibbs-Helmholtz relation

$$\Delta G^\circ_{ads} = \Delta H^\circ_{ads} - T\Delta S^\circ_{ads} \qquad (3.16)$$

where, ΔG°_{ads} = Change in free energy of adsorption; ΔH°_{ads} and ΔS°_{ads} = Change in enthalpy and Change in entropy; T = Temperature.

The plot of free energy of adsorption as a function of temperature was drawn. The slopes of these lines are equal to ΔS°_{ads}, and the intercepts on free energy axis give the corresponding change of enthalpy (ΔH°_{ads}) **(Eddy *et. al.,* 2010)**.

3.3.2 Electrochemical Methods

All the experiments were carried out in the double walled glass cell of capacity 200 mL having provisions for the inlet of nitrogen gas, working electrode (MS), counter platinum electrode and luggin capillary. The potential of the working electrode was measured with respect to saturated calomel electrode (SCE) through luggin capillary. The experiments were carried out after the steady state attainment of corrosion potentials (15 mts) at 30 ± 1°C. For the electrochemical techniques, **SOLARTRON ELECTROCHEMICAL MEASUREMENT UNIT (1280B)** model interfaced with an IBM computer was used with a software package of ZPLOT 2 and CORR WARE 2. The polarization studies were made after the specimen attained a steady state potential. The potential was carried out from a cathodic potential of -0.2V to an anodic potential of +0.2V with respect to the corrosion potential at a sweep rate of 0.5mV/s. E versus log I curves were plotted. AC impedance measurements were done in the frequency range of 20 KHz to 0.1Hz. The charge transfer values were obtained from the plots of Z' and Z". The values of (R_t+R_s) corresponds to the point where the plot cuts Z' axis at low frequency and R_s corresponds to the point where the plot cuts Z' axis at high frequency. The difference between R_t and R_s gives the charge transfer resistance (R_{ct}) values. The C_{dl} values were obtained from the relationship **(stated in ASTM, G 1-2, and 1996b)**.

$$C_{dl} = \frac{1}{2\Pi f_{max}} \times R_{ct} \qquad (3.17)$$

where, C_{dl} = double layer capacitance; R_{ct} = charge transfer resistance; f_{max} = frequency at Z' value maximum.

Measurement of Corrosion Current (I_{corr})

Values of corrosion currents were obtained by Tafel extrapolation method. In Tafel extrapolation method, plots of η vs log current were made and on extrapolation gave the corrosion current and the slope if the linear portion of the anodic and cathodic curves gave b_a and b_c respectively **(Jeyapraba *et al.,* 2006)**.

Determination of Inhibition efficiency

The inhibition efficiency was obtained from the equation:

$$\text{Inhibition efficiency (\%)} = \frac{I_{corr(blank)} - I_{corr(inh)}}{I_{corr(blank)}} \times 100 \qquad (3.18)$$

where, $I_{corr\ (blank)}$ = corrosion current in the absence of inhibitor; $I_{corr\ (inh)}$ = corrosion current in the presence of inhibitor.

Besides the above method, the inhibition efficiencies were obtained from R_p and R_{ct} values as follows,

$$\text{Inhibition efficiency (\%)} = \frac{R_{p(inh)} - R_{p(blank)}}{R_{p(inh)}} \times 100 \qquad (3.19)$$

$$\text{Inhibition efficiency (\%)} = \frac{R_{ct(inh)} - R_{ct(blank)}}{R_{ct(inh)}} \times 100 \qquad (3.20)$$

where, R_p and $R_{ct(inh)}$ = polarization resistance and charge transfer resistance in the presence of inhibitor; $R_{p(blank)}$ and$R_{ct(blank)}$ = polarization resistance and charge transfer resistance in the absence of inhibitor.

Calculation of Surface Coverage (θ)

Surface coverage from impedance measurements was calculated using the formula **(Jeyaprabha *et al.*, 2005)**

$$\text{Surface Coverage } (\theta) = \frac{C_{dl(blank)} - C_{dl(inh)}}{C_{dl(blank)}} \qquad (3.21)$$

where, $C_{dl\,(blank)}$ = the double layer capacitance in the absence of inhibitor; $C_{dl\,(inh)}$ = the double layer capacitance in the presence of inhibitor.

3.3.3 Surface Analytical Techniques

3.3.3.1 FT-IR Spectral Analysis

FT-IR was recorded using BRUKER Optik GmbH FT-IR spectrometer MODEL No – TENSOR 27 with the SOFTWARE – OPUS version 6.5 (CECRI – India) which extended from 4000 and 400 cm^{-1} for corrosion products adsorbed on the surface of MS.

3.3.3.2 Scanning Electron Microscope

To study the topography of the iron substrate after corrosion in the presence and absence of the inhibitor the instrument **JEOL MODEL JSM 6360** was used.

3.3.4 Molecular modeling /Quantum chemical approach /Computational details

Quantum-chemistry calculations have been widely used to study the reaction mechanisms and to interpret the experimental results as well as to solve chemical ambiguities. This is an useful approach to investigate the mechanism of reaction in the molecule and its electronic structure levels. The structure and electronic parameters can be obtained by means of theoretical calculations **(Ebenso *et al.*, 1996).**

This QSAR approach is adequately sufficient to forecast the inhibitor effectiveness using the theoretical approach; it may be used to find out the optimal group of parameters for predicting a molecule's suitability to be a corrosion inhibitor. There is no doubt that the recent progress in DFT has provided a very useful tool for understanding molecular properties and for describing the behaviour of atoms in molecules. All the computations and calculations were carried out using **Gaussian 03 code of programs using 6-31G (d).** Exchange and correlation calculations were carried out with the functional hybrid B3LYP and the 6-31G (d) orbital basis sets for all the atoms. In all cases, total structure optimization together with the vibrational analysis of the optimized structures was carried out in order to determine whether they correspond to a maximum or a minimum in the potential energy curve. The frontier molecular orbitals, namely, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are evaluated for 2-Methoxy-4-methylphenol, 2-Methoxy phenol, 2,6-Dimethoxy phenol and Phenol using the following equations.Ionisation potential (IP) and electron affinity (EA) were calculated from E_{HOMO} and E_{LUMO}

$$\text{Ionisation potential (IP)} = -E_{HOMO} \tag{3.22}$$

$$\text{Electron Affinity (EA)} = -E_{LUMO} \tag{3.23}$$

In DFT, the ground state energy E(ρ) of an atom/molecule can be expressed in terms of its electron density. Using the finite difference approximation, the global softness σ can be evaluated. The global hardness η, which is the inverse of the global softness can be evaluated using the following equations: **(Parr and Yang, 1989; Chattaraj *et al.*, 2007)**.

$$\text{Energy gap } (\Delta E) = E_{HOMO} - E_{LUMO} \tag{3.24}$$

$$\text{Global Hardness } (\eta) = \frac{E_{HOMO} - E_{LUMO}}{2} \tag{3.25}$$

$$\text{Global Softness } (\sigma) = \frac{1}{2\eta} \tag{3.26}$$

$$\text{Electronegativity } (\chi) = \frac{IP + EA}{2} \tag{3.27}$$

$$\text{Electrophilic Index } (\omega) = \frac{\mu^2}{2\eta} \tag{3.28}$$

where, E_{HOMO} = Highest occupied molecular orbital; E_{LUMO} = Lowest unoccupied molecular orbital; μ = Dipole moment.

Two strategies are followed for the computation of the above-mentioned parameters: the first is the energy-vertical method, which is based on the difference in total electronic energies when an electron is added or removed with reference to the neutral molecule. The second is based on the difference between the HOMO and the LUMO energies of the neutral molecule and is known as the orbital-vertical method.The aim of this investigation is to compute the relevant electronic properties by means of DFT model chemistry to generate accurate information that enables better understanding of the inhibitory behaviour exhibited by CN and BF phenolic compounds. In this investigation, the geometrical features of the four main compounds present in CN/BF extracts are studied theoretically. In order to explain the inhibitory performance of these phenolic compounds, the O–H BDE and electronic properties such as HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) energies, ionization potential (IP), electron affinity (EA), hardness (η), softness (S), electronegativity (χ) and electrophilic index (ω) are computed and analyzed in detail.

3.4 WORK PLAN

Work plan carried out in the current investigation is depicted in the flow chart

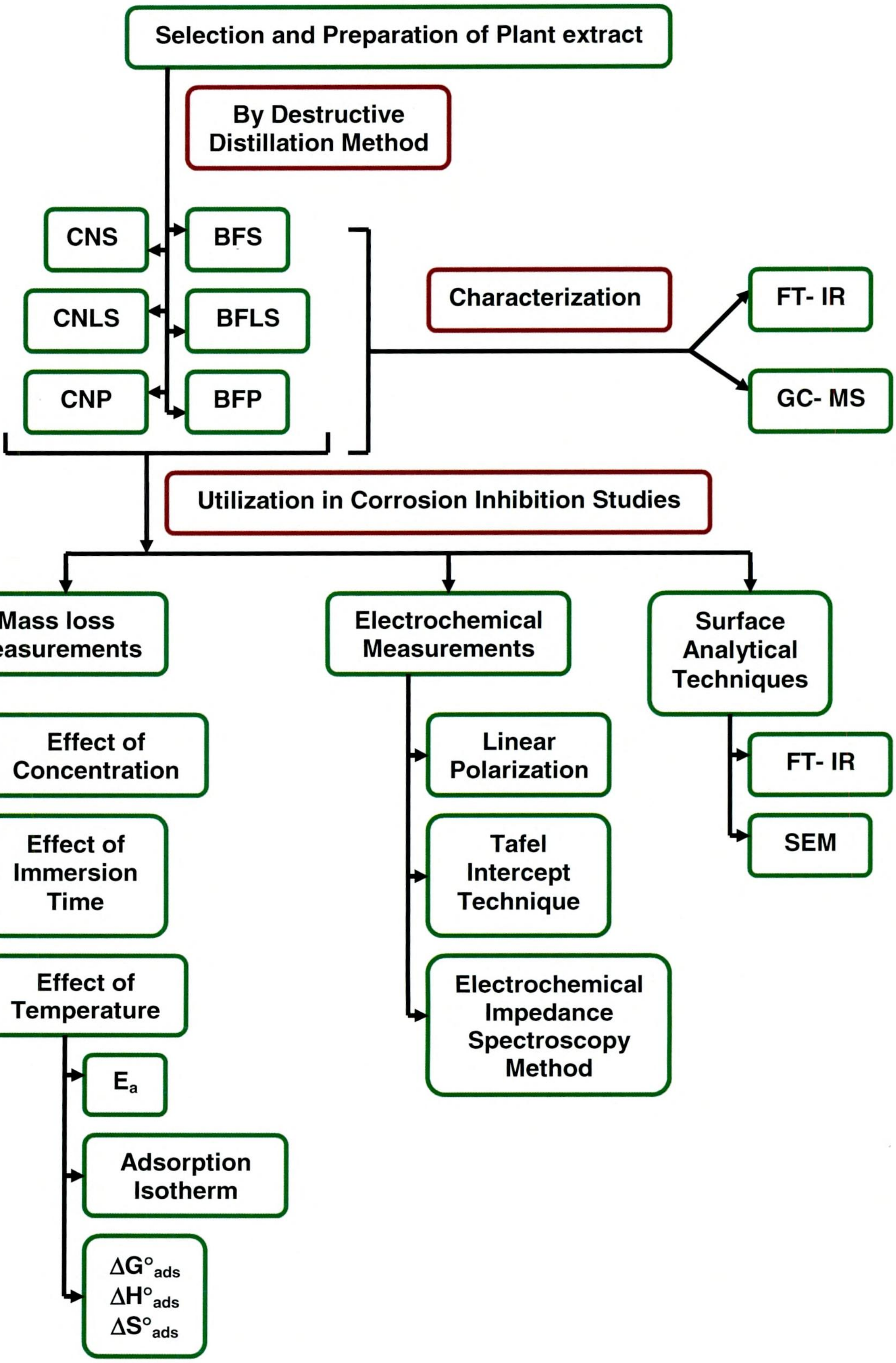


Figure – 15 Work plan

3.5 INSTRUMENTS USED

List of instruments handled is represented in Figure-16.

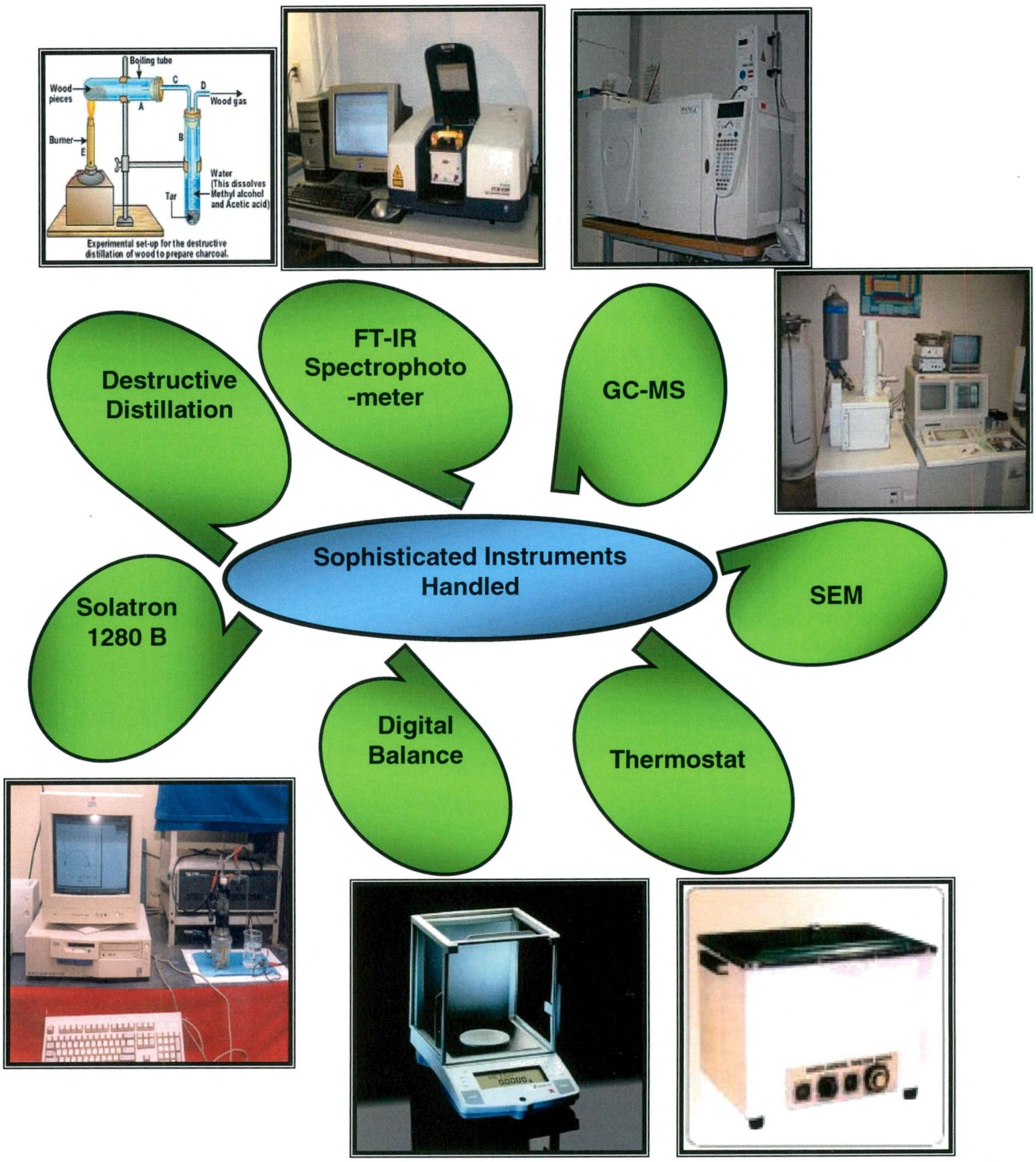


Figure - 16 Sophisticated Instruments handled