Chapter 3: Materials and Methodology

This section is categorised into four subsection. First section incorporates the backhand principle of Aspen plus wherein all the basic equation working simultaneously are listed in the section 3.1. Second subsection includes the Aspen plus Modelling Approach and the methodology adopted to perform the simulation work and the sensitivity analysis. Third section includes the materials and methodology adopted for the experimental investigation. This section also include all the technical details of the equipment used while performing experimental work. Last subsection includes the methodology adopted to perform the RSM based multi-objective optimization analysis. This section also includes the block diagram and the flowchart to obtain optimized parameters.

3.1 Backhand Principle of Aspen plus

Aspen plus is mainly based on the concept of minimizing Gibbs free energy to predict syngas composition and gasification performance. At the equilibrium conditions, Gibbs free minimization [86] is defined as:

$$G^t = \sum_{i=1}^{N} n_i \mu_i \quad (1)$$

Where n_i and μ_i denote total mole concentration and chemicals potentials of i^{th} species respectively. The ideal gas response of gas is defined as:

$$\mu_i = G_i^0 + RTln\left(\frac{f_i}{f_i^0}\right) \quad (2)$$

Where T and R denote temperature and gas constant. f_i represents fugacity of i^{th} species. G_i^0 and f_i^0 represents standardized Gibbs free energy and the standardized fugacity of i^{th} species. Equation 2 can be transformed in the form of pressure and it is depicted in equation 3

$$\mu_i = G_i^0 + RTln\left(\frac{\Theta P_i}{P^0}\right) \quad (3)$$

Where Θ denotes fugacity coefficient. It is seen from the experimental analysis that the magnitude of f and P attains the same value as the pressure tends to attain null value. Due to this, real gas tends to behave like an ideal gas. At this condition equation 3 can be transformed as:

$$\mu_i = \Delta G_{f,i}^0 + RTln(y_i) \quad (4)$$

Where y_i denotes the mole frac of i[th] species whereas $\Delta G_{f,i}^0$ depicts the standardized Gibbs free energy of formations of i[th] species. It is generally kept 0 for all chemical reactions. On substituting equation (4) in equation (1), equation 5 is obtained:

$$G^t = \sum_{i=1}^{N} n_i \Delta G_{f,i}^0 + \sum_{i=1}^{N} n_i RTln\left(\frac{n_i}{n_{tot}}\right) \quad (5)$$

The main purpose is to search for the magnitude of a set of n_i for which the magnitude of Gibbs free energy is at a minimal point. Elemental balance constraint is defined as:

$$\sum_{i=1}^{N} a_{ij}\, n_i = A_j \quad (6)$$

Where a_{ij} denotes atom of a j[th] element in a mole of the i[th] species and A_j defined as the cumulative j[th] element in a mixture. Gibbs free energy can be minimalized by incorporating Lagranges multipliers. It is depicted in equation 7.

$$\frac{\delta L}{\delta n_i} = \Delta G_{f,i}^0 + n_i RTln\left(\frac{n_i}{n_{tot}}\right) + \sum_{j=1}^{k} \varepsilon_j\, a_{ij} \quad (7)$$

Where L is Langranges multiplier and ε_j is the Langrage multiplier. This equation deals with the minimization of Gibbs free energy approach.

3.2 Aspen plus Modelling Approach

The complete air gasification process including pre-treatment and post-treatment was simulated using ASPEN PLUS V10. The process of air gasification was simulated by developing a new kinetic free thermochemical equilibrium model. Complete modeling of the air gasification process was segregated into four phases: biomass drying, biomass decomposition, biomass gasification, and producer gas filtration. The first phase deals with the drying operation where the moisture content of biomass is reduced to the ideal level before feeding into the reactor. The drying operation was computed by incorporating a user-programmed external FORTRAN sub-routine statement in the calculator block. In the second phase, pre-dried biomass is decomposed into its elemental form. Volatile components and char were also generated in this phase. The yield distribution for these components was regulated by the FORTRAN statement. The third phase deals with the partial oxidations and the governing gasification reactions by decreasing Gibbs free energy to the minimum level. The fourth phase deals with the post-treatment operation where the solid components were separated from the syngas using a cyclone separator. Finally, producer gas is cooled down to produce clean syngas.

3.2.1 Property package

The inbuilt IDEAL property method has been preferred for the simulation. This property package is selected because the processes involved during the simulation includes the conventional constituents at high temperature. Hence, this property package is best suited for this simulation. Biomass was described as the non-conventional components by using the chemical properties of the feedstock. It is because different constituents of biomass were not defined in the inbuilt Aspen Plus library. The enthalpy and density model incorporated for biomasses were HCOALGEN and DCOALIGT respectively. MCINCPSD stream type was

preferred because of the presence of both conventional and non-conventional streams in the process.

3.2.2 Assumptions

The following assumptions are considered for the simulation process. [87]

- Kinetic free, steady-state, stoichiometric, and isothermal model.
- Tar contents and other heavy hydrocarbon are neglected.
- All gases are considered Ideal gases.
- Carbon and ashes are considered as the mere composition of char.
- The complete concentration of sulfur reacts to form H_2S.
- No NO_X is produced except NH_3.

Table. 3.1 Explanation of Aspen plus operating block used for modeling.

Aspen Plus Default ID	**Assigned ID**	**Descriptions**
RStoich	DRIER	Reduces moisture content from biomass.
Flash2	DEMOIST	Segregate the wet air from the dried biomass.
RYield	DECOMP	Perform decomposition operation analogous to pyrolysis process.
Mixer	MIXER	Mix air with decomposed elemental constituents
RGibbs	GASIFICA	Perform a gasification process using 3 phase equilibrium
SSplit	CYCLONE	Segergrates the solid particles from the hot gas.
Heater	COOLER	Reduces the temperature to ambient

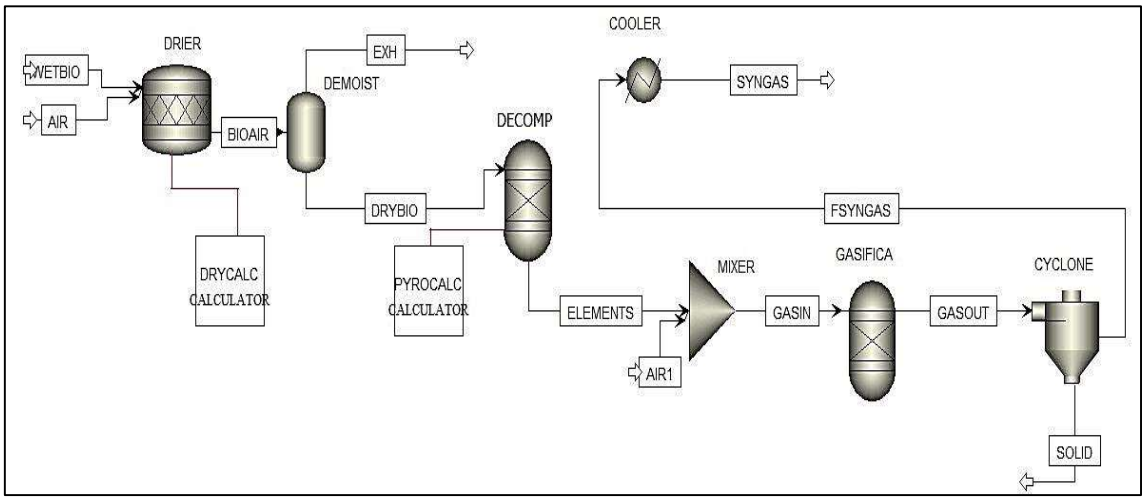

Fig. 3.1. Schematic layout of the biomass gasification process in ASPEN PLUS

3.2.3 Development of ASPEN Plus model

Seven ASPEN Plus inbuilt operation blocks were used to model and simulate the complete air gasification processes (see table 3.1). Figs 3.1 and 3.2 depict the ASPEN Plus simulation flowsheet and its block diagram of calculation procedure respectively. The stream 'WETBIO' was identified as the raw wet biomasses before the operation of Drayng. It was described as the non-conventionals components associated with the input of Proximate and Ultimate analysis. In the present model, 'WETBIO' and 'AIR' were discharged to 'DRIER' for the drying of wet biomasses. RStoich block in ASPEN Plus was termed as 'DRIER'. The 'DRIER' was regulated by the external user-programmed FORTRAN subroutine statements named 'DRYCALC' in the calculator block. It is to downgrade the magnitude of the moisture contents in biomass to a specific point. After this, the dried out biomasses along with air having moisture was discharged to 'DEMOIST' through a stream named 'BIOAIR'. 'DRIER' and 'DEMOIST' together simualtes drying phase. Dried biomass and wet air were segregated by the 'DEMOIST'. 'EXH' was discharged into the ambient surrounding whereas 'DRYBIO' was sent to the 'DECOMP' reactor.

RYield inbuilt reactor in the ASPEN Plus block was termed as the 'DECOMP'. This reactor was taken into account when the product distribution was well-identified but the kinetics and reaction stoichiometries were unidentified. The main objective of the 'DECOMP' reactor in the simulation was to decompose the dried non-conventionals biomasses into its elemental constituents, like C, H_2, O_2, S, N_2, Moisture, and ASH. 'DECOMP' reactor simulates pyrolysis phase. The decomposition of non-conventional biomass is important as Gibbs free energy of non-conventional components could not be computed by the simulator but it can be calculated after decomposing it into its elemental form. This decomposition was controlled by the external user-programmed 'PYROCALC' FORTRAN statement. This calculator uses the dried biomass ultimate analysis data to calculate the product distribution. Decomposed components coming out from the 'DECOMP' reactor through the stream named 'ELEMENTS' was then blended with ambient air through the stream 'AIR1' in a mixer named 'MIXER'. It was then discharged to the 'GASIFICA' reactor through the stream 'GASIN'. RGibbs inbuilt reactor in the ASPEN Plus database was termed as 'GASIFICA'. This reactor is used to create the thermo-chemical equilibrium compositions between products and reactants. It is also used where the reaction stoichiometry was unidentified but the pressure and temperature of the reactions were known. The oxidation and reduction zone of the reactor was simulated by the 'GASIFICA' reactor by decreasing Gibbs's free energy to the lowest point. Reactions (R7-R11) was the governing reactions in this reactor to predict the PG composition coming out from the reactor through the stream named 'GASOUT'.

The Producer gas named 'GASOUT' was then sent to the separator 'CYCLONE'. This separator is used to segregate the solid component from the gas mixture through the stream 'SOLID'. The other outlet stream coming out from topside 'FSYNGAS' was comprised of all the combustible gases and moistures coming out from the separator 'CYCLONE'. It was further cool down to the surrounding temperature by 'COOLER'. Due to the cooling effect, the

moisture content in 'FSYNGAS' was condensed. 'CYCLONE' and 'COOLER' together simulates producer gas filtration. and Eventually, clean fuel can be obtained named 'SYNGAS' through the process of thermochemical conversion of biomass i.e. gasification.

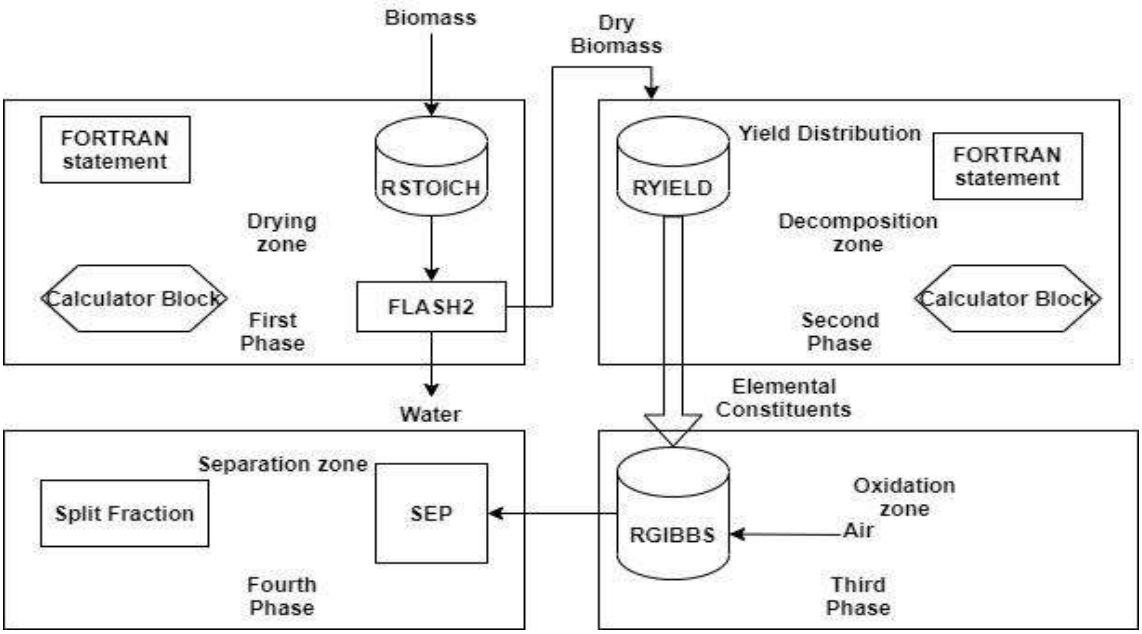

Fig. 3.2. Block Diagram of ASPEN Plus simulation for the different zone of a gasifier

3.3 Experimental Methodology

3.3.1 Test fuels

To conduct the experiment, the biomass and Non-woody biomass had been procured from the local market of Varanasi, Uttar Pradesh in India, which belongs to the open cast mine of Madhya Pradesh and Bihar state mines.

The gasifier-ICE experimental setup consists downdraft gasification system comprised of a reaction chamber with a thermocouple integrated, blower, air control valve, scrubber, cyclone separator, test flare, water pump, three-chamber for fine filtering system, and integrated with

compression ignition (CI) engine. The schematic diagram of the gasifier-ICE setup is shown in Fig.3.3. The photograph of the Gasifier unit is shown in Fig.3.4, and its details are shown in table 3.2. The engine is facilitated with variable compression ratio (VCR), and comprised with direct injection, water-cooled, naturally aspirated engine, eddy current dynamometer, and governor controlled 1500 engine rpm. The detailed specification of the engine is mentioned in table 3.3. The characteristics of engine combustion and performance were recorded on a computer through the integration software-Engine Soft. The photograph of the VCR Engine set up is shown in Fig.3.5. Orifice and manometer were used to measure the air and gas flow rate separately.

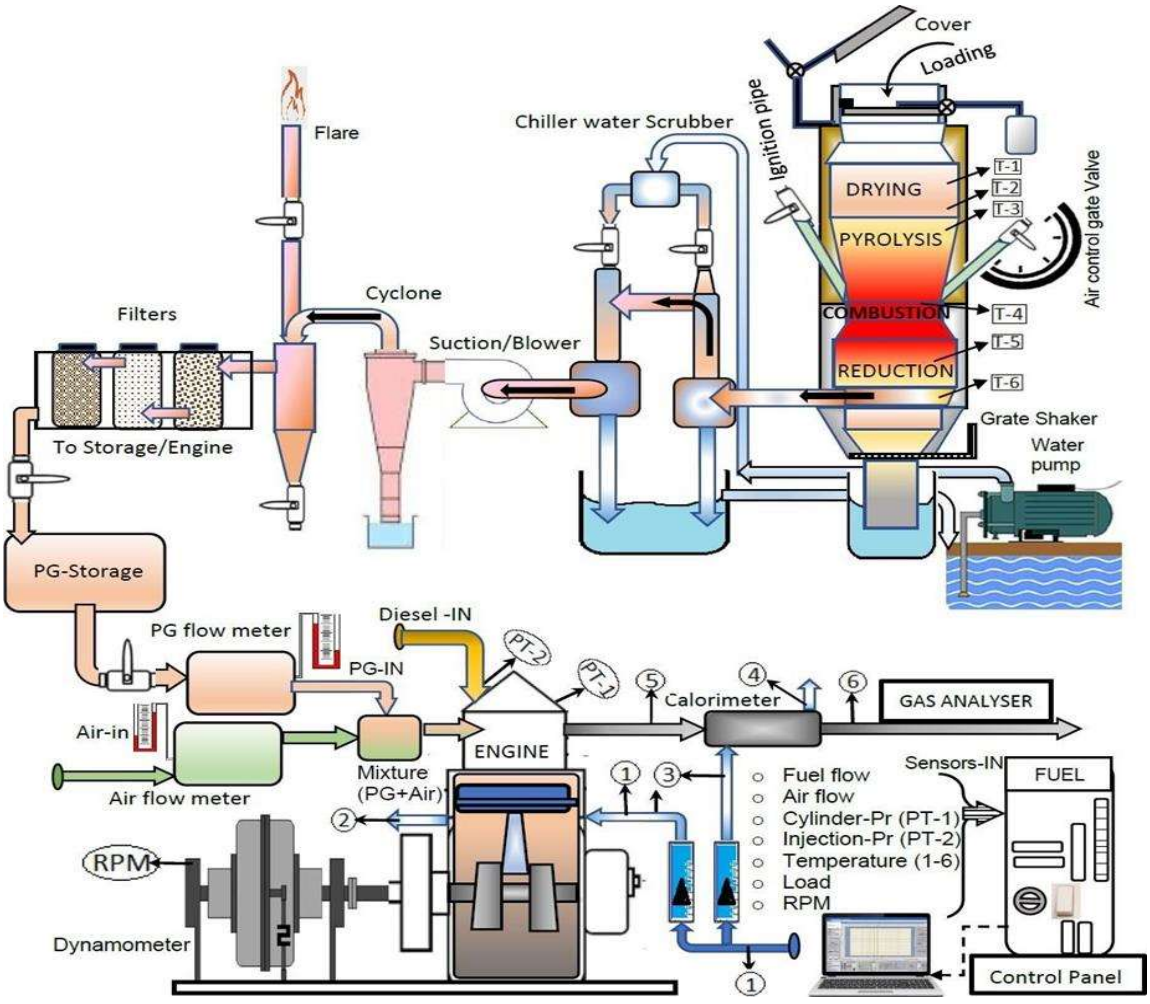

Fig. 3.3. Schematic of the downdraft gasifier-CI engine experimental setup unit

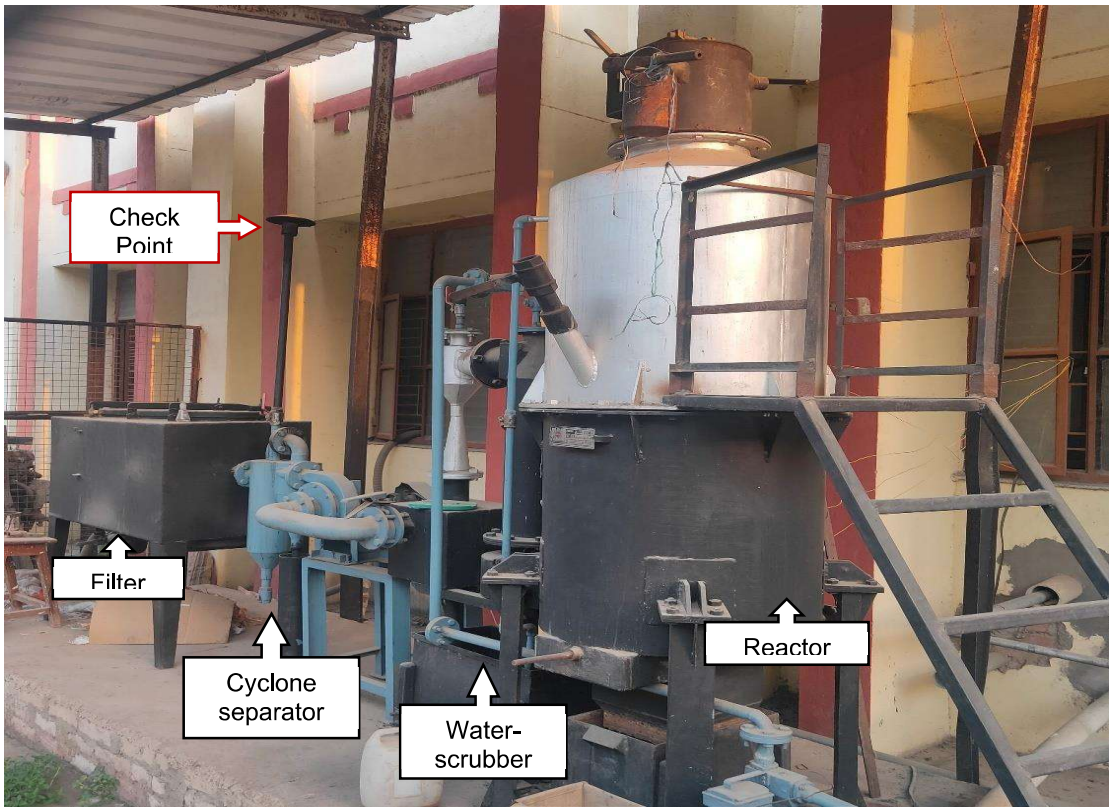

Fig. 3.4. Photograph of Downdraft gasifier experimental setup

Table. 3.2. The detailed specification of Gasifier

Particular	**Description**
Type of gasifier	Downdraft
Made	Urja Gasifier
Reactor	Conical shape
Gasification agent	Air
Operating pressure	Atmospheric
Rated power	14 kW
Rated Fuel consumption	6 kg/h
Rated gas flow	15 Nm^3/h
Air supply system	Two nozzles
Hopper storage capacity	40 kg
Temperature	800-900 ^0C
Feeding system	Manual loading coupled with hopper
Discharge system	Grate and ash box
Startup	Through blower

Table.3.3. Technical Specifications of Engine

Particular	Description
Model	Kirloskar, 240PE
Engine type	Single cylinder, VCR, 4 stroke CI engine
Compression ratio	12:1-18:1
Bore (Diameter)	8.75 cm
Stroke length	11.0 cm
Cooling system	Water-cooled
Rated power	3.5 kW at 1500 rpm
Dynamometer	Eddy current (water cooling) coupled with loading unit
Load sensor	Strain gauge (0 to 50 kg)
Airflow transmitter	Pressure transmitters,
Fuel flow transmitter	DP transmitter,
Rotameter	Engine cooling 40-400 LPH, calorimeter 25-250 LPH
Software	Enginesoft

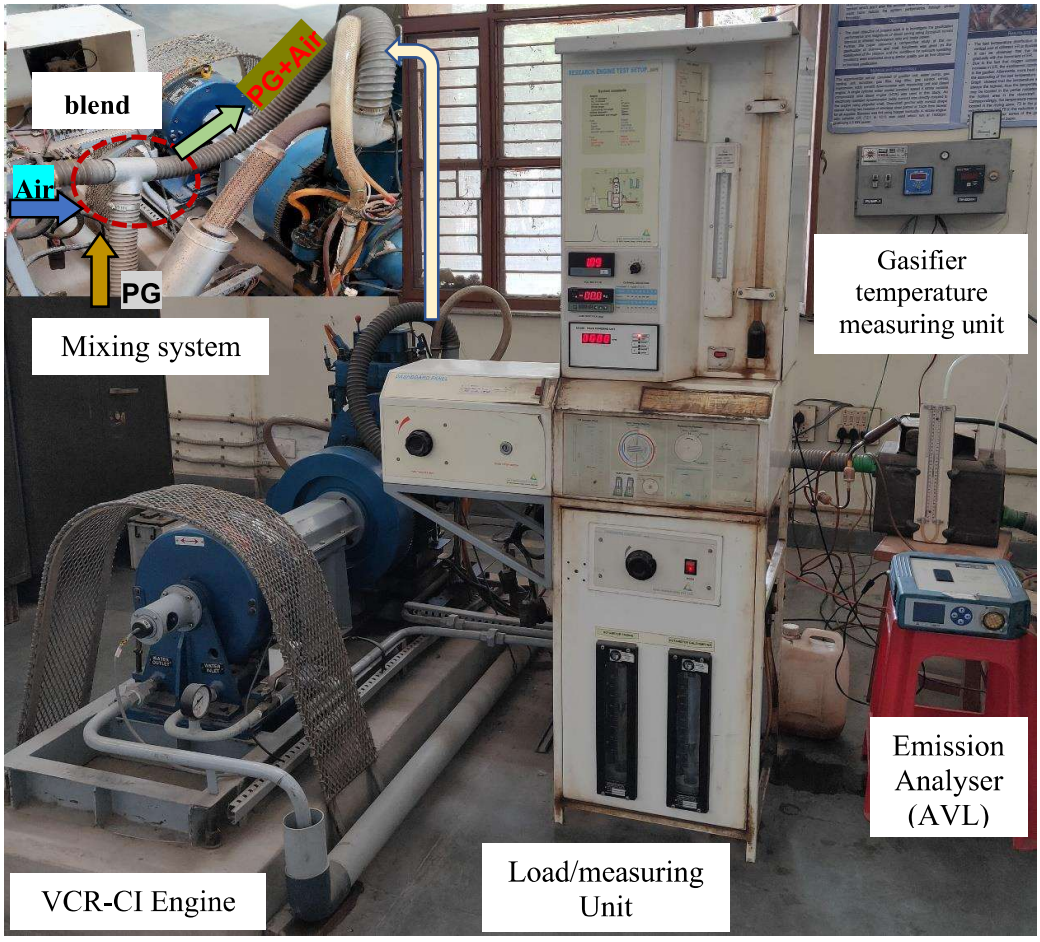

Fig. 3.5 Photograph of the VCR IC engine testbed in lab

3.3.2 Experimental setup and procedure

The ICE experimental analysis has been conducted followed by producer gas generation from hard coke-low grade Coal and biomass gasification (Fig.3.3,3.4). To do this, initially, the coal/biomass feedstock was loaded into the gasifier reactor through a hopper placed at the top opening, and little kerosene was sprayed near to the ignition point for quick burning. Thereafter, the air blower was turned on for the suction of air from the nozzle into the combustion zone. The flame was kept near both the nozzle port for catching fire to the feedstock. After a certain time, when coal had been little red hot and temperature reached around 500 ^{0}C and beyond at oxidation reaction zone, the valve opened, and producer gas (PG) allowed to go for water-based scrubbing, cyclone separating, and filtration. Firstly, in the scrubbing and cooling section, PG passes through a water scrubber where the PG temperature reduces toward ambient temperature, and circulating water tries to remove the contaminants which are soluble in water like SO_2 (Sulphur dioxide) and Hydrogen Sulphide (H_2S) from the PG, and also tar, soot particles, etc. from the PG. Besides, PG passed through a cyclone separator for further cleaning. Henceforward, frequently the flammability of producer gas was checked at the checkpoint until the testing flame changes it's colored and develops flare. It was observed that near to 650 ^{0}C the testing flame changed its color and developed a flare. Thereafter, producer gas was allowed to pass through three-chamber filtration units (Rice husk, wood dust, and heavy cotton cloth) in a sinusoidal trajectory. Then, Producer gas emerging out from the filtration unit, possessing temperature in the range of 35-55 ^{0}C, was allowed to enter the PG storage, to mixing chamber where PG mix with air in the desired proportion, and to the control, the valve then to the inlet section of Engine.

Henceforward, VCR engine performance and emission had to be investigated. For the comparative analysis of engine performance between conventional Diesel and dual-fuelled of PG and Diesel, initially, the experiment was conducted with diesel mode only to investigate

engine performance, fuel consumption and emission with different compression ratios (15,16,17,18) and load variation (0 to12 kg) at fixed 1500 rpm. Subsequently, dual fuel mode engine operation was conducted to measure engine performance and emission characteristics at different compression ratios and load. In addition to this, the effect of gasifier equivalence ratio due to nozzle opening on the engine performance characteristics was measured. The equivalence ratio (ER) is the ratio of the mass of the actual fuel-air ratio to the stoichiometric fuel-air ratio in the gasification. It changes when the throat of the gasifier nozzle valve opens, partial oxidation reaction inside the gasifier increases, and thus the heating value of syngas compositions changes. The producer gas flow rate was measured by the airbox U tube manometer method. Thermal performance characteristics data like diesel consumption, brake power, BSFC, pressure drop all were observed and recorded using the "enginesoft" software. After collecting data from single and dual-mode engine runs, the response surface method (RSM) was applied to optimize the engine performance, specific fuel consumption, and emission corresponding to the input variable of CR, Load, and Blending percentage.

3.4 Optimization Methodology

Response surface methodology (RSM) is considered as the best design of experiment (DOE) methods. It has multiple applications in different segments of the engineering field. The main work of this technique is the simultaneous optimization of the variable objective. Thus, the multi-objective optimizations approach using RSM has been incorporated for this present investigation. Fig 3.6 depicts the comprehensive flow diagram of the RSM solving methodology.

The main utilization of RSM is to develop a regression model equations between the independent decision variables and the output response through analysis of variance (ANOVA) tool. In the present study, RSM was employed for determining the optimum performance independent parameters, quadratic effect, the main effect, and interaction effect of operating

parameters (Temperature, Equivalence ratio). CCD (central composite design) having (α = 1.414) was adopted. There were 13 runs were executed in ASPEN Plus which include 4 corner point, 4 stars/ axial point, and 5 centered points. The coded value of 600,700,750,800, and 900^{0}C temperature and 0.2, 0.4, and 0.6 ER were marked as -1, 0, and +1 respectively. The interconnection between the independent variable and response is represented by the polynomial quadratic equation [88]

$$y = \beta_0 + \sum_{i=1}^{n} \beta_i x_i + \sum_{i=1}^{n} \beta_{ii}\, x_i^2 + \sum_{i=1}^{n-1} \sum_{j=1}^{n} \beta_{ij} x_i\, x_j + \varphi \qquad (1)$$

where y is output response, x is decision parameters, β is coefficients, n is the number of factors, and φ is a statistical error.

The quantification of the regression model's efficiency is quantified by R^2_{adj} parameter. This parameter is acquired from the ANOVA tool. It is calculated as follows [88]

$$R^2_{adj} = 1 - \left(\frac{\frac{SOS_R}{(n-p)}}{\frac{SOS_T}{(n-1)}} \right) = 1 - \frac{(n-1)}{(n-p)} (1 - R^2) \qquad (2)$$

Where the sum of the square of the residual (SOS_R) and the total of the sum of squares is calculated as follows [88]

$$SOS_R = \sum_{i=1}^{n} \left(y_i - y_j \right)^2 \qquad (3)$$

Where, y_i and y_j are observations and fitted observations.

$$SOS_T = \sum_{i=1}^{n} y_i^2 - \frac{(\sum_{i=1}^{n} y_i^2)}{n} \qquad (4)$$

R^2 is computed using the following equation [88]

$$R^2 = 1 - \frac{SOS_R}{SOS_T} \tag{5}$$

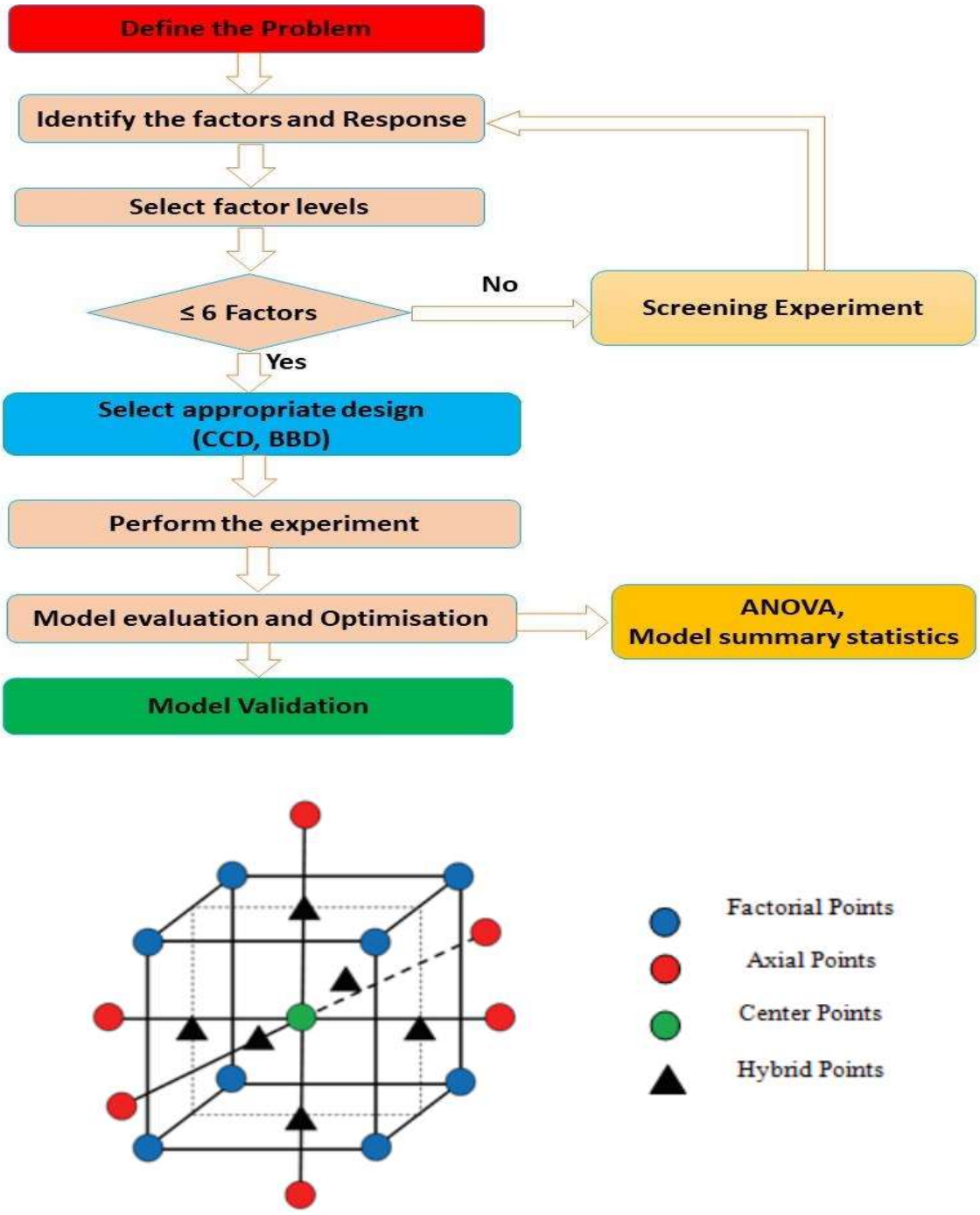

Fig. 3.6 Flow diagram of RSM solving methodology and CCD factorial design