

CHAPTER 4

DESIGN & SIMULATION

The understandings from literature review and pre-research study are incorporated to identify the research gap. The findings of the pre-research study have verified the necessity of designing a waste heat recovery device specifically for HEVs. The scientific principles of thermionic energy conversion have also emphasized the possibility of such a device with a maximum economy and efficiency. Here, the intended function of a proposed Thermionic Regeneration System (TRS) is verified and validated with the help of its design & simulation. This chapter represents the processes carried for the designing and simulation of a TRS.

Designing is an establishment of a product to perform the desired functions. The product is either entirely new in abstraction, performing a new type of work, or it is more economically performing the work that can be done by existing product. It is an advancement or magnification of an existing product for improved economy and proficiency. A TRS design represented in this research is formulated by integration of two methods. One is the finalization of conceptual design and other is the reverse engineering. A conceptual design is used to form a baseline structure satisfying basic principles and requirements of a thermionic conversion. Whereas the reverse engineering is adopted to redesign an existing automotive component as a TRS by integrating conceptual design, without effecting its existing performance. The design is then simulated using a multiphysics simulation software.

Simulation generally refers to the modeling of a design, in such a way that it performs its desired functions on a virtual platform. A software based simulation is a computer program that is derived from the required input parameters for the working of a product. Simulation is commonly used for design verification & to improve the control parameters & features. It also verifies the logic with which a product is simulated. These virtual environments are created with the help of scientific and mathematical expressions as well as the experimental findings from the previous research. It becomes simple and cost effective to analyze the behavior of a product using simulation in comparison to direct experimentation. A TRS design is simulated for its power output & conversion efficiency using thermionic emission module on a multiphysics software.

The design methods and simulations carried in this research are explained in the sections below;

4.1. Conceptual Design of a Thermionic Regeneration System (TRS)

Thermionic energy conversion is comprised of principle of thermionic emission derived from Richardson Dushman's equation. The technical information from the description of a thermionic energy conversion have accentuated the key elements for the design. A novel design is produced by recognizing the functions of the key elements of thermionic conversion. The configuration of design is combination of such elements however it is unique for automotive application. Calculations are carried out to establish the size of each element in order to verify that the basic criteria of each piece are met. These measurements are crucial in the design of a thermionic regenerator. The basic procedure used for the design of thermionic regenerator consists of the following levels:

Level 1. Specify the elements & their function

Level 2. Identify available elements and their feasibility in design

Level 3. Prepare a conceptual design for prototyping

Level 4. Select suitable material for prototyping

Level 5. Determine geometric dimensions of the elements for conceptual design

Level 6. Prepare working drawing of the elements

Level 1: Specify the elements & their function

A design of thermionic regenerator is incorporated with seven basic elements. The specification of each element's functions is the first step in the design process. The function of elements are as follows (The elements are shown in Figure 4.1):

- 3) Top Fixture: This element holds the collector & insulator at the specified position from top.
- 4) Insulator: An insulator is used to maintain electrical and thermal insulation between emitter and collector.
- 5) Top Guide: This element holds the emitter & insulator at the specified position from top
- 6) Emitter: It is an electrode which heats & emits electrons.
- 7) Collector: It is an electrode which collects the emitted electrons.
- 8) Bottom Guide: This element holds the emitter & insulator at the specified position from top
- 9) Bottom Fixture: This element holds the collector & insulator at the specified position from bottom.

Level 2. Identify available elements and their feasibility in design

The elements for thermionic regenerator mentioned above are specially considered for development. Therefore it is convenient to identify existing products which will perform the required function. A proposed shape of thermionic regenerator is a cylindrical one where the most critical element of the thermionic regenerator becomes its insulator.

An insulator must satisfy the function as well as its design should be in a cylindrical shape. In order to develop an insulator especially for the thermionic regenerator would be an expensive and time consuming process. Hence, the available insulator products were searched for the same. Finally, it is found that, a borosilicate glass tube is a good insulator, also it is in cylindrical shape.

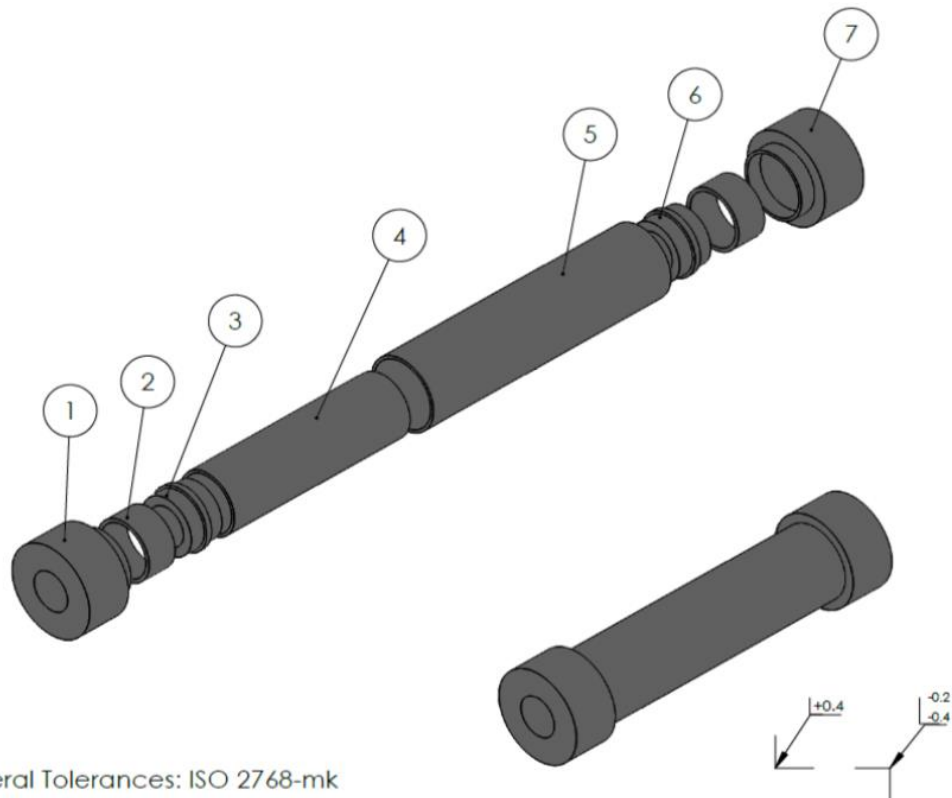
Emitter and collector are determined as per the insulator dimensions. As per the literature survey the best suitable materials for emitter and collector are tungsten and molybdenum. Tungsten and molybdenum are available in rod form.

The guides and fixtures for top and bottom of a thermionic regenerator are supporting elements and needed to be developed as per the size of an emitter collector and insulator using machining.

Level 3. Conceptual Design of a small scale Thermionic Regenerator

The thermionic regenerator must satisfy following design considerations:

- 1) Lower inter electrode gap: It is understood from the literature survey that inter electrode spacing plays an important role in electron transfer from emitter to collector. A small scale thermionic regenerator is designed for an inter electrode gap of 0.5mm (achievable with machining).
- 2) Electrical insulation: Along with the gap emitter and collectors are required to be insulated from each other. A glass insulator is designed to facilitate electrical insulation between emitter and collector.



General Tolerances: ISO 2768-mk

Fig. 4.1. Exploded View of a designed Thermionic Regenerator (Kodihal & Sagar, 2019a)

The seven elements described in Level 1 are arranged in such a way that a cylindrical shape of thermionic regenerator is achieved. The designed thermionic regenerator is a small scale for prototyping (i.e. for proof of concept) as shown in Fig. 4.1. General machining tolerances are considered.

Level 4. Select suitable material for prototyping

The thermionic emission properties of the collector and emitter materials must be good. The work function of the material determines the efficiency of TEC. The work function of a material is a measurement of its ability to emit electrons at a certain temperature. It represents the amount of energy necessary for a metal to emit electrons. The temperature at which electrons are released decreases as the work function decreases.

The Materials selected for the parts are mentioned in Table 4.1. These materials are for the prototyping purpose only. Where for emitter and collector tungsten and molybdenum are considered for the final product.

A borosilicate glass used in chemical labs is taken by considering its ability to resist heat and provide electrical insulation. The glass insulator is a base element considered while designing other elements.

Table 4.1. Assembly Design Part Description (Kodihal & Sagar, 2019a)

Sr. No	Part	Material	Details
1	Top Fixture	Mild Steel	It Fixes The Position Of Collector At Top
2	Insulator	Borosilicate Glass	Provides Electrical Insulation
3	Top Guide	Mild Steel	Separates Emitter To Maintain Gap (0.5 mm) from Top
4	Emitter	Mild Steel, Al, Brass, Tungsten	21×68×1mm (Dia×Length×Thickness)
5	Collector	Mild Steel, Al, Brass, Molybdenum	24×92×1mm (Dia×Length×Thickness)
6	Bottom Guide	Mild Steel	Separates Emitter To Maintain Gap (0.5 mm) From Bottom
7	Bottom Fixture	Mild Steel	It Fixes The Position Of Collector At Bottom

Level 5. Determine geometric dimensions of the elements for conceptual design

The shape of the thermionic regenerator is determined by the operating conditions and the shape of the adjacent element. Because cylindrical shape was a fundamental necessity. The adjacent elements must have a cylindrical shape. The glass insulator, tungsten & molybdenum rod availability where considered for determining the dimensions of other elements.

Available tungsten & molybdenum rods are in 12.7mm (1/2 inch) to 101.6mm (4 inch) in diameter. Whereas available borosilicate glasses are in 4mm to 325 mm in diameter and 0.5mm to 9mm thickness. The test method for analysis needs an experimental setup on which the heating and inter-electrode potential measurement can be done. These all measurements will be conducted using Arduino as a data acquisition tool. Hence the parameters for selecting the dimensions of insulator, emitter & collector are; availability of element, the minimum surface area through which a measurable thermionic conversion is easily possible and low cost. Considering these parameters following dimensions are finalized.

Assumptions:

Assuming that Arduino UNO has 10-bit ADC, when we select the Analog reference to be 5V, its resolution is $5/2^{10}=5/1024=0.0048828125$ V. So the minimum voltage we can read is 0.0048828125 V. whereas maximum voltage for measurements is taken here as 6V. The material constants are taken for tungsten and molybdenum.

Design Calculations:

1) Finding the minimum surface area for thermionic emission:

- Total Electrical power output

$$E_{output} = V \times I$$

Where,

V is the voltage

I is current

The expected electrical power output is 45 W at the current rate of 7.5 amp/hr.

Now, the current density can be given as;

$$I = J \times A$$

Where,

J is current density

A is surface area

As the current density & surface area are unknown, Current density through thermionic emission is given as,

$$J_{th} = AT^2 \exp \frac{-\Phi}{k_B T}$$

Where,

J= Current Density A/mm²

T= Emitter Temperature

Φ= Emitter Work Function

A= Richardson Constant

K_B= Boltzmann's constant i.e. (8.6173 × 10⁻⁵)

$$J_{th} = 20(1073.15)^2 \exp \frac{-(4.5)}{(8.6173 \times 10^{-5})1073.15}$$

$$J_{th} = 14.48 \frac{A}{m^2}$$

Hence, Surface area is, $A = \frac{I}{J}$

$$= \frac{0.0724}{14.48}$$

$$\mathbf{A = 5179.55 \text{ mm}^2}$$

(Here a minimum current output i.e. 0.0724 amp is considered.) The available tungsten rod as an emitter is having **21 mm** outer diameter. Hence for the surface area of 5179.55 mm². A height of a cylinder will be;

$$A = 2\pi rh + 2\pi r^2$$

$$5179.55 = 2\pi (10.5) h + 2\pi (10.5)^2$$

$$\mathbf{h = 68 \text{ mm}}$$

For electric potential of 6 V the inter-electrode gap can be calculated by child's law,

$$J = \frac{KV_d^{\frac{3}{2}}}{d^2}$$

Where,

K is the child's constant i.e. 0.0023340

V is the voltage

J is the current density

d is the inter-electrode gap in mm

$$d^2 = \frac{KV_d^{\frac{3}{2}}}{J}$$

$$d^2 = \frac{0.0023340 \times (6)^{\frac{3}{2}}}{14.48}$$

$$d^2 = 0.208$$

$$\mathbf{d = 0.4578 \text{ mm}}$$

Hence, the emitter dimensions are;

$$D \text{ (Outer Diameter)} = 21 \text{ mm}$$

$$d \text{ (Inner Diameter)} = 19\text{mm}$$

$$L \text{ (Length)} = 68 \text{ mm}$$

To maintain inter-electrode gap of 0.5 mm approx., the Collector dimensions are;

$$D \text{ (Outer Diameter)} = 24 \text{ mm}$$

$$d \text{ (Inner Diameter)} = 22 \text{ mm}$$

$$L \text{ (Length)} = 92 \text{ mm}$$

Corresponding to that as per the design an insulator dimensions are;

$$D \text{ (Outer Diameter)} = 20 \text{ mm}$$

$$d \text{ (inner Diameter)} = 18 \text{ mm}$$

$$L \text{ (Length)} = 15 \text{ mm}$$

Level 6. The dimensions of other elements are taken as shown in 2D drawings from Fig. 4.2 to Fig 4.8.

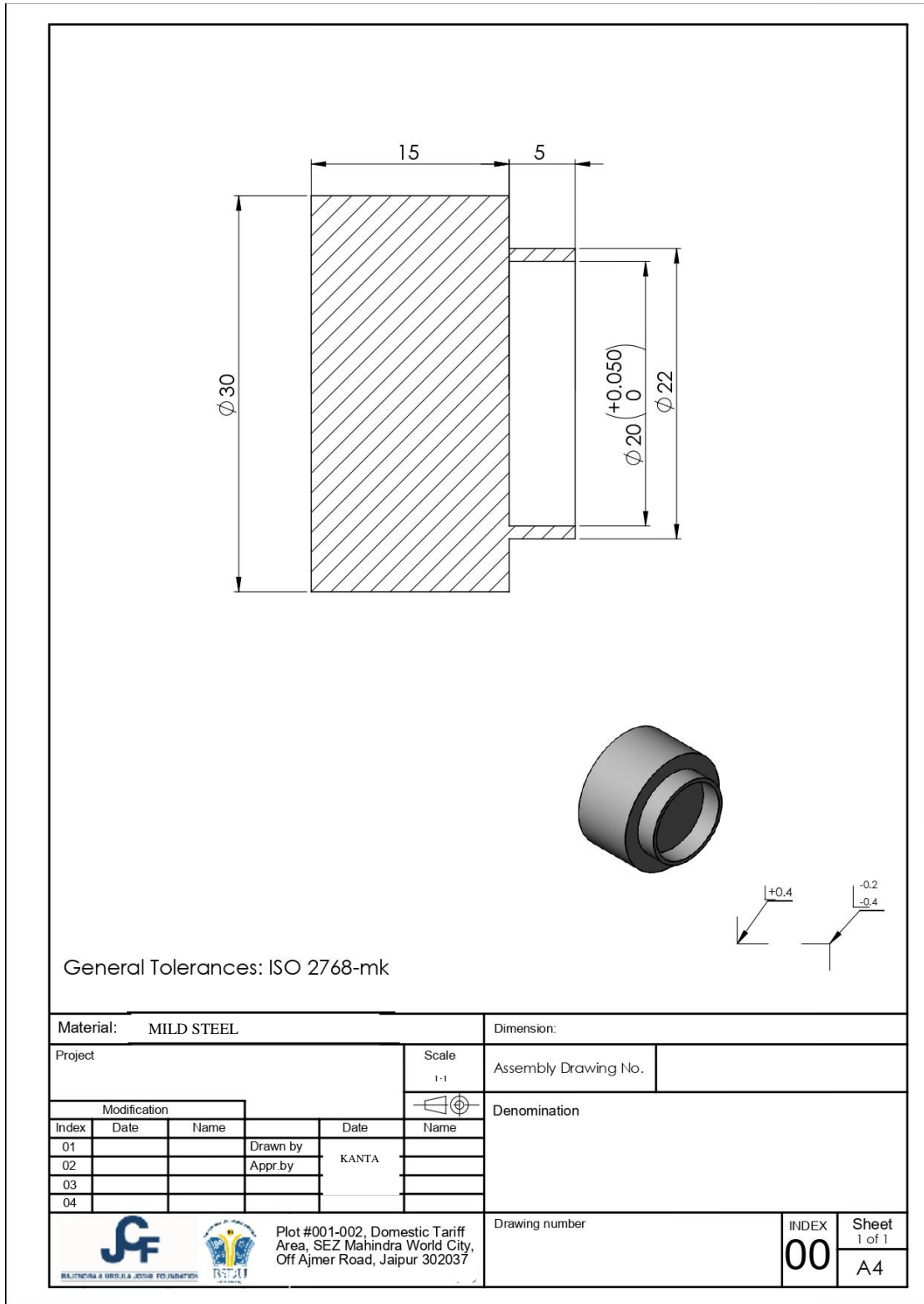


Fig. 4.2. Bottom Fixture

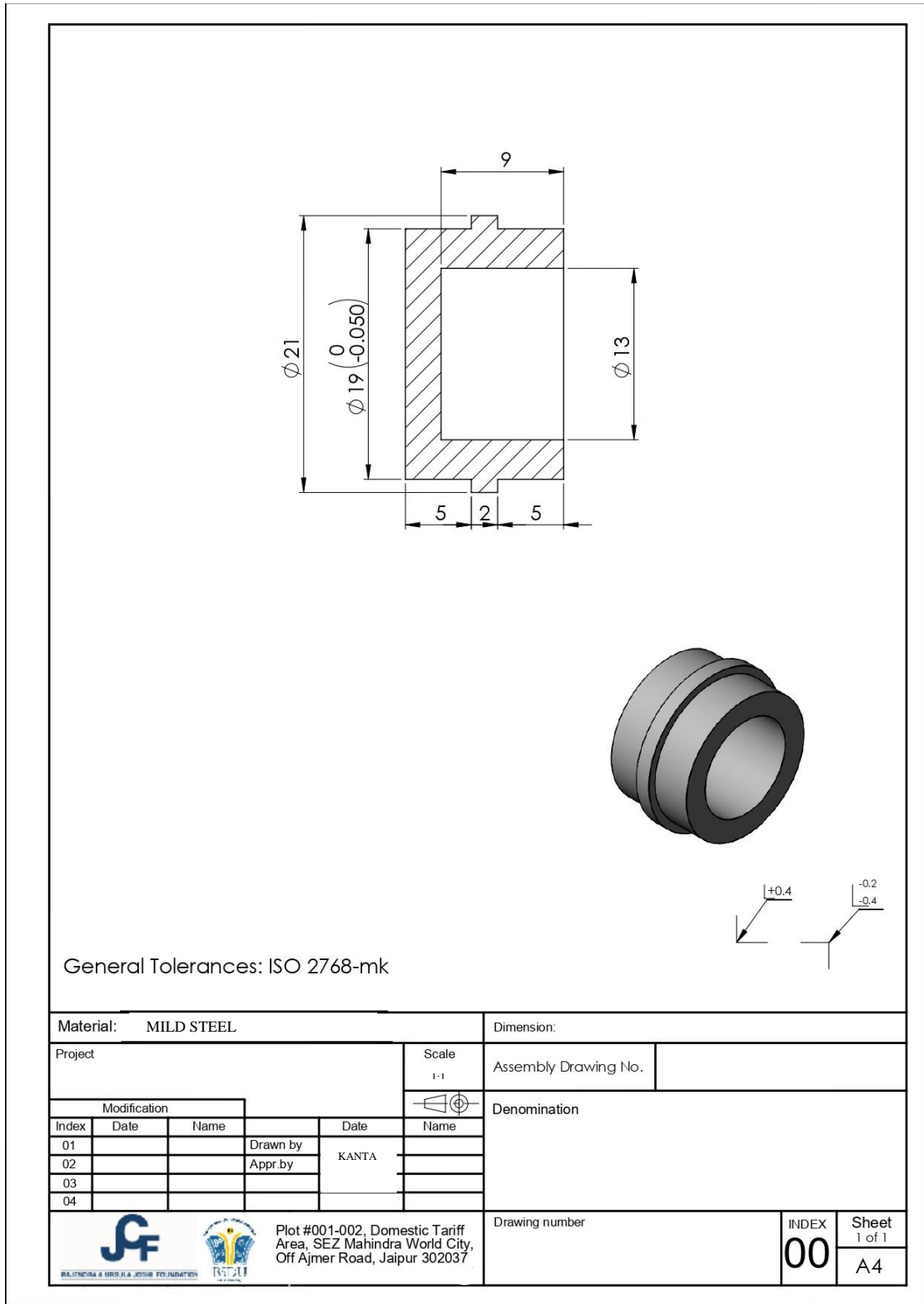
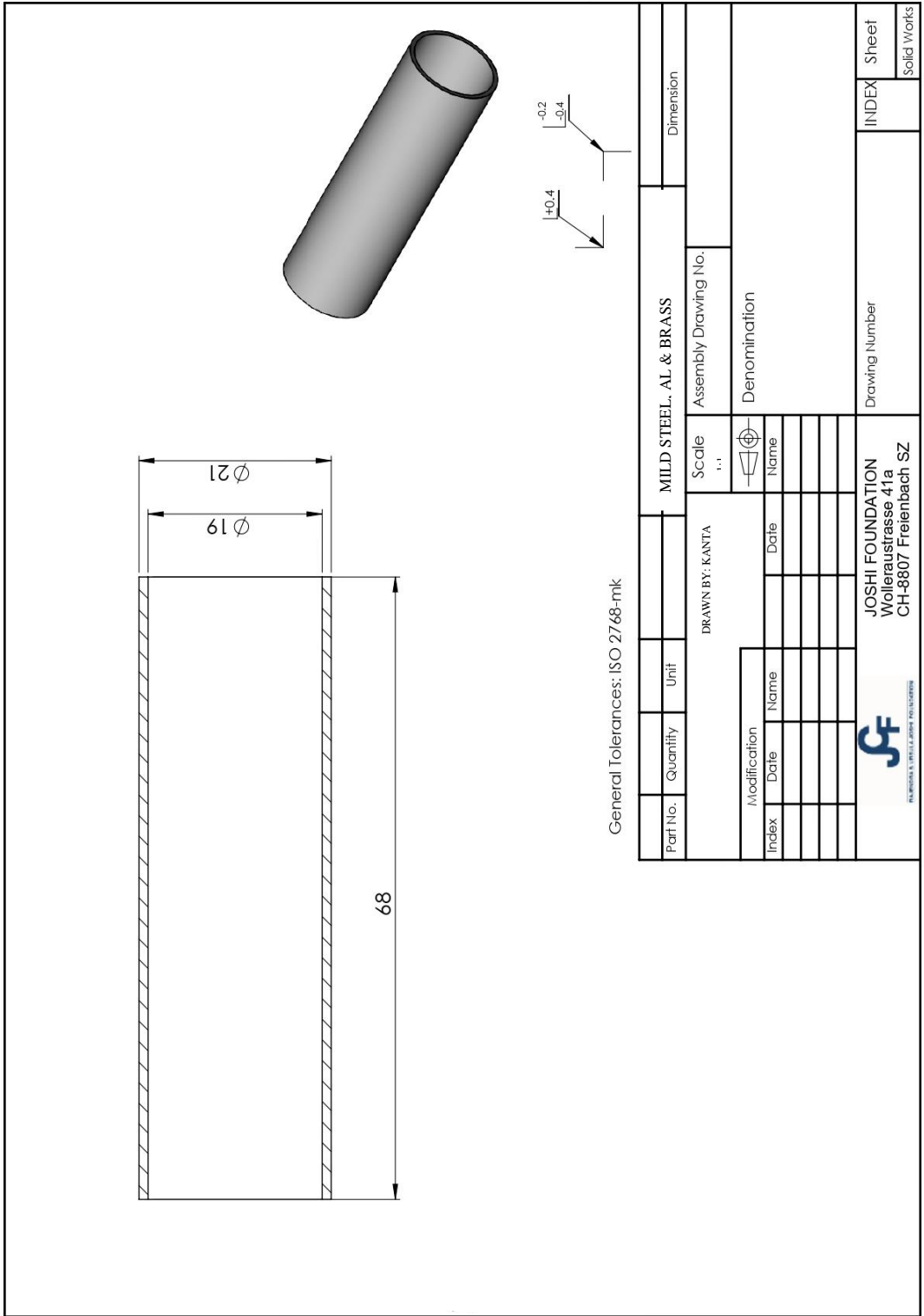


Fig. 4.3. Bottom Guide



General Tolerances: ISO 2768-mk


Part No.	Quantity	Unit	MILD STEEL, AL & BRASS	Dimension
DRAWN BY: KANTIA			Assembly Drawing No.	
Scale 1:1			Denomination	
Modification	Date	Name		
Index	Date	Name		
	Date	Name		
	Date	Name		
	Date	Name		
 <small>JOSHIA & COMPANY FOUNDATION</small>			Drawing Number	
JOSHI FOUNDATION Wajirastrasse 41a CH-8807 Freienbach SZ			INDEX	Sheet
				Solid Works

Fig. 4.4. Emitter

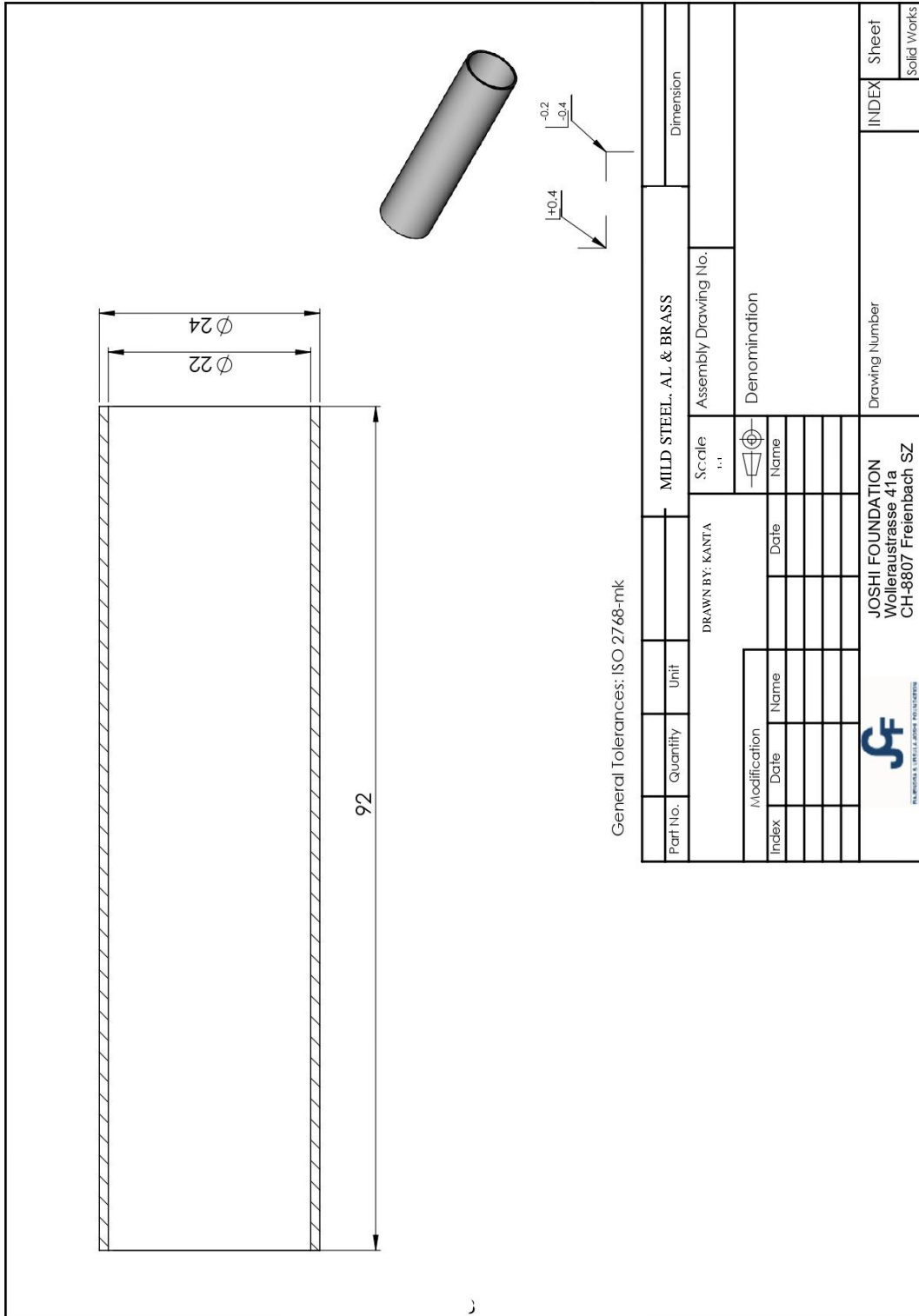


Fig. 4.5. Collector

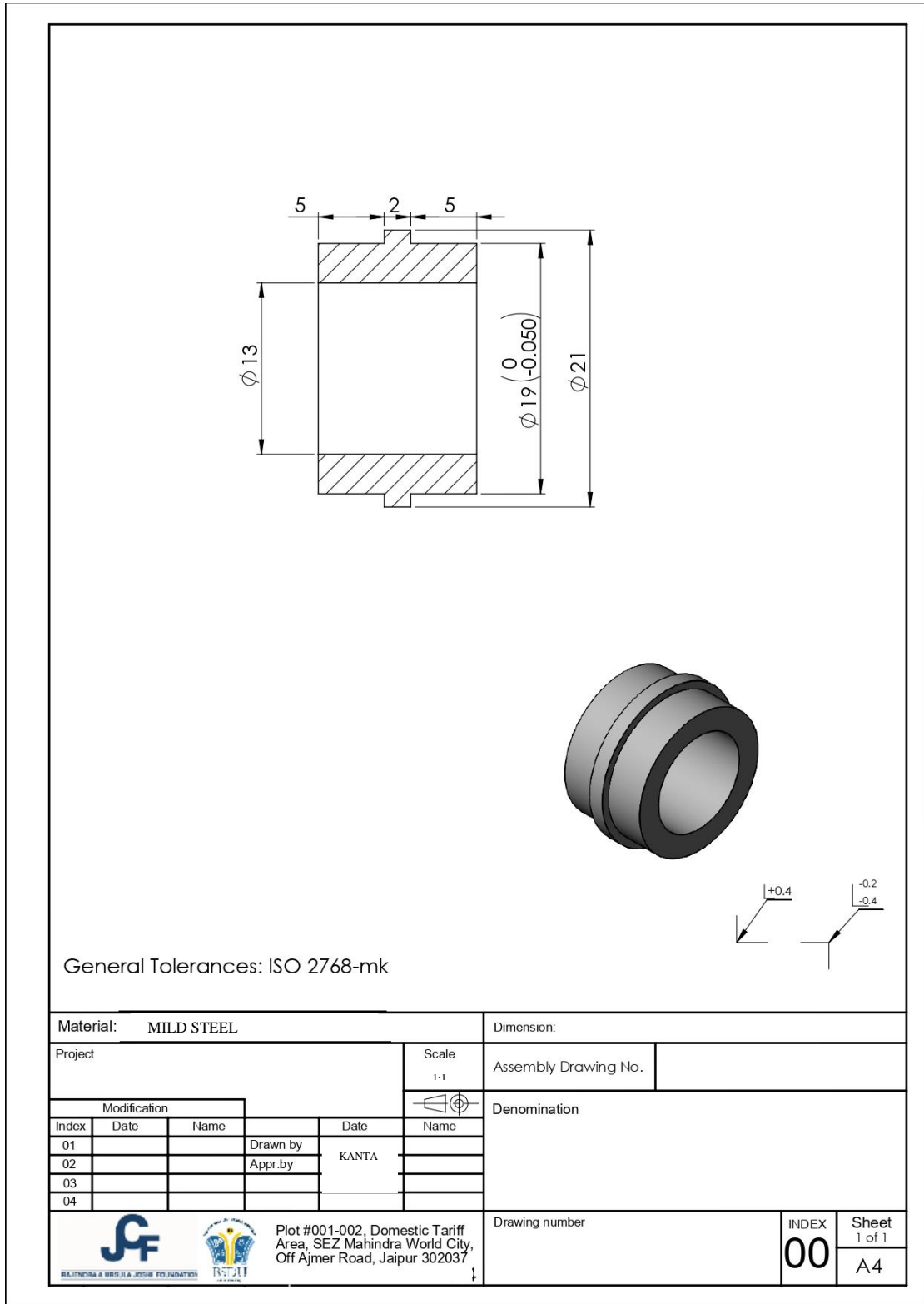


Fig. 4.6. Top Guide

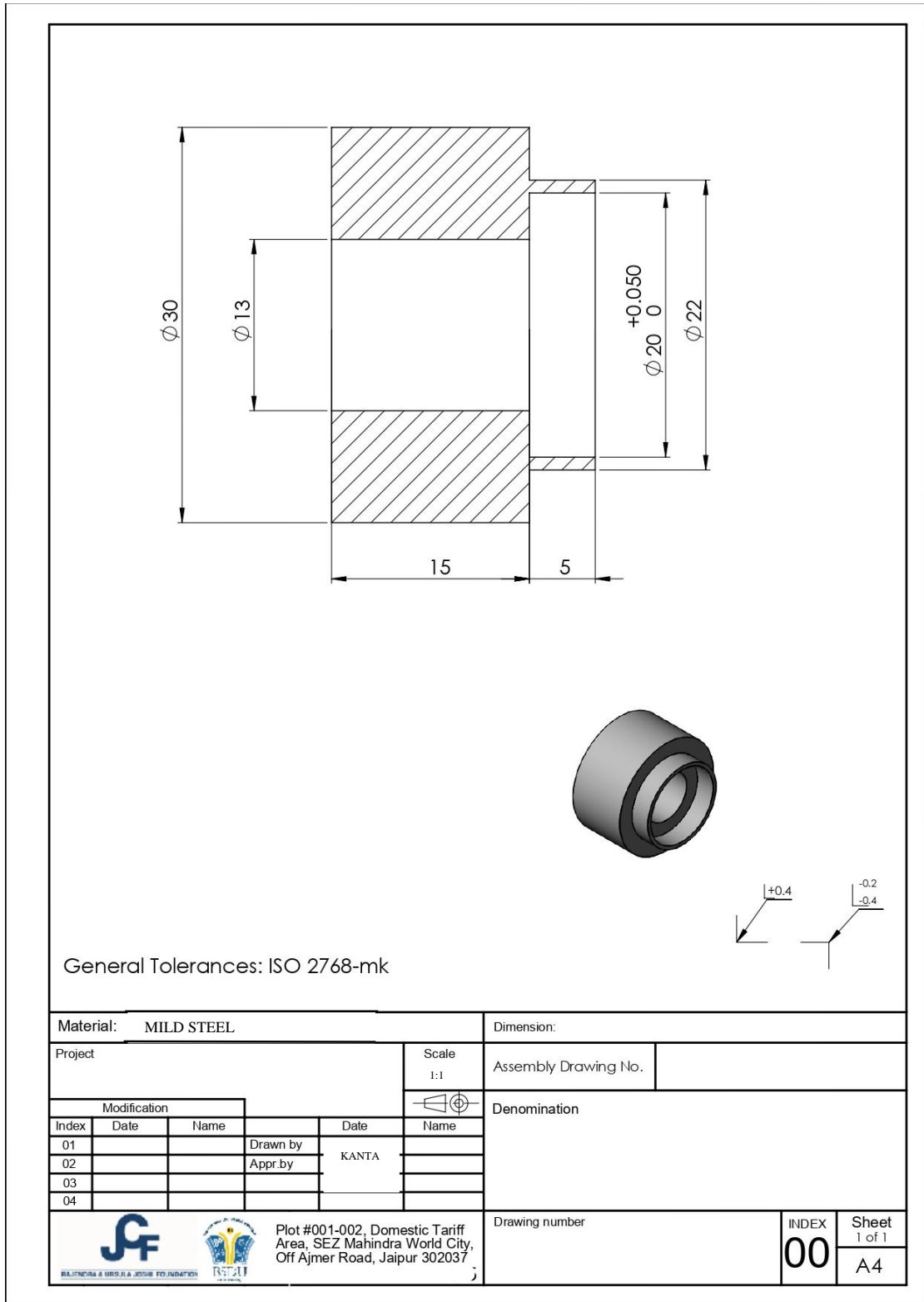


Fig. 4.7. Top Fixture

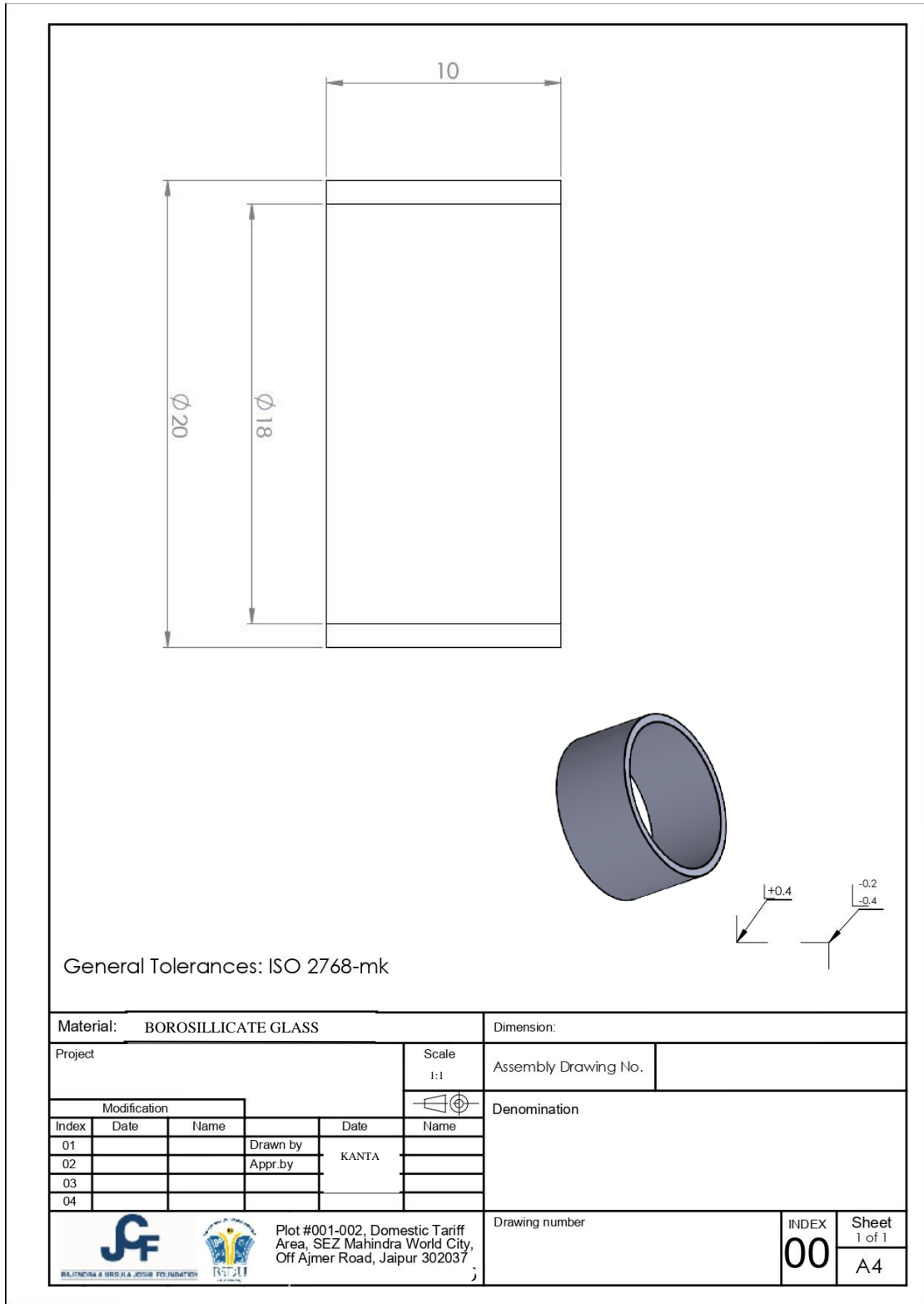


Fig. 4.8. Insulator

4.2. Reverse Engineering

The conceptual design shown in above section is a small scale design whereas the objective of this research is to develop a design for automotive application. In order to do so a reverse engineering methodology is used to redesign the model for large scale application.

Automotive engine generates heat through combustion of fuel. A portion of the heat is turned to mechanical energy for work, while the rest is transferred to the cylinder walls, exhaust, and other engine components. Hence in order to recover this transferred heat in useful energy i.e. electrical, the engine components are needed to be redesigned so that the component itself can act as heat to electricity generator.

The engine components from where heat is lost are; cylinder liner, cylinder block, exhaust manifold/tailpipe, engine mechanical components such as piston, connecting rod, crank etc. The waste heat analysis of an automotive engine shown in section 3.1 highlights that total 60% of the heat is lost. According to the literature (Spitsov, 2013) 15-20% of heat is lost in cooling system, 20-30 % is lost through exhaust gases and 5-10% heat is lost through other mediums like metal surfaces and through radiation. Form this it is understood that a cylinder liner and exhaust manifold/ tailpipe are the components from where maximum energy can be recovered.

Therefore reverse engineering of cylinder liner is carried out using coordinate measuring machines (CMM). Computer aided design (CAD) data of a cylinder liners of Mahindra 1.5 lit & 2.2 lit diesel engines and one exhaust manifold is taken from CMM. Fig 4.9 shows the 3D design obtained after CMM measurements.

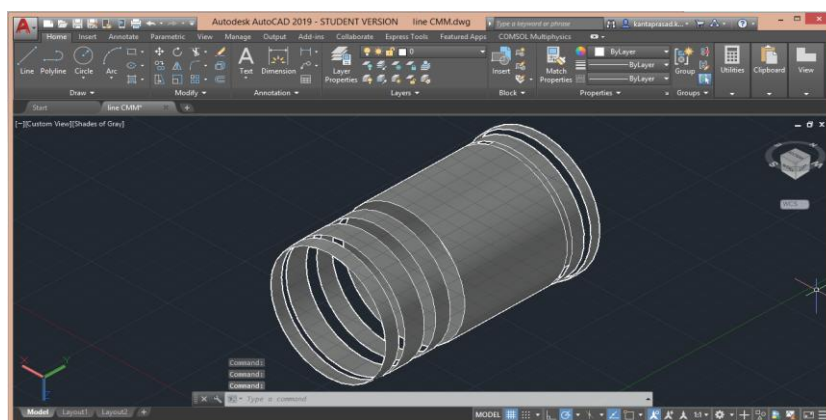


Fig. 4.9. Obtained CAD Design from CMM

The CMM measurements for cylinder liner dimensions were compared with the conceptual design to understand the feasibility in redesigning. Designing each and every component of thermionic regenerator as in the dimensions of a cylinder liner needs following major modifications;

- 1) Redesigning the cylinder block: Changing the design of a cylinder liner needs major change in design of a cylinder block.
- 2) Redesigning cooling jackets and wall thickness of liner: The cooling jackets and wall thicknesses must be redesigned.
- 3) Reconsidering materials: As the cylinder liner material needs to perform thermionic emission also, the materials consideration will also be a critical part.
- 4) IC engine performance: The performance of an IC engine depends upon the internal pressure developed during compression and that is achieved by a good cylinder liner. Hence maintaining engine's performance unaffected is also a critical part.

This shows that redesigning of a cylinder liner is a complicated and not feasible for converting it as a thermionic regenerator. Compared to this an exhaust system is more feasible for redesigning and therefore taken for CMM measurements. Therefore an exhaust pipe is taken for measurements as shown in Fig. 4.10 & Fig 4.11.



Fig. 4.10. Exhaust pipe taken for measurement



Fig. 4.11. Measurements on CMM

The Fig. 4.12 shows the obtained CAD data points of the exhaust pipe cut section using CMM. The same dimensions are considered while developing TRS model in above simulations. Table 4.2 shows the obtained CAD data from CMM measurements.

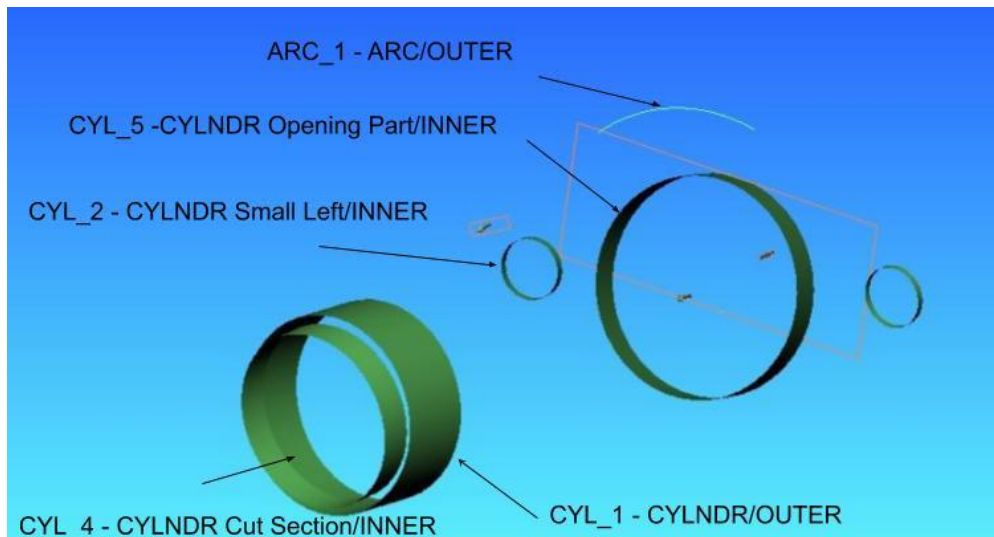


Fig. 4.12. CAD Drawing Obtained from CMM for exhaust pipe

Table 4.2. CMM CAD Data for exhaust pipe

Cyl_1 - Cylindr/Outer						
Label	Nominal	Actual	Deviation	Lower Tol.	Upper Tol.	Oot
Diam	38.0000	38.1500	0.1500	0.0000	-0.1000	0.2500
Cyl_2 - Cylindr Small Left/Inner						
Label	Nominal	Actual	Deviation	Lower Tol.	Upper Tol.	Oot
Diam	11.6900	11.6900	0.0000	0.0000	-0.1000	0.1000
Cyl_4 - Cylindr Cut Section/Inner						
Label	Nominal	Actual	Deviation	Lower Tol.	Upper Tol.	Oot
Diam	34.0400	34.0400	0.0000	0.0000	-0.1000	0.1000
Cyl_5 - Cylindr Opening Part/Inner						
Label	Nominal	Actual	Deviation	Lower Tol.	Upper Tol.	Oot
Diam	41.9800	41.9800	0.0000	0.0000	-0.1000	0.1000
Arc_1 - Arc/Outer						
Label	Nominal	Actual	Deviation	Lower Tol.	Upper Tol.	Oot
Diam	35.2700	35.2700	0.0000	0.0000	-0.1000	0.1000
Distb_1 - Distb/Nominal,Pt2pt (Pla_1 - Pla_2)						
Label	Nominal	Actual	Deviation	Lower Tol.	Upper Tol.	Oot
Diam	2.0262	2.0269	0.0007	0.0000	-0.1000	0.1000
Distb_2 - Distb/Nominal,Xaxis (Cyl_5 - Cyl_2)						
Label	Nominal	Actual	Deviation	Lower Tol.	Upper Tol.	Oot
Diam	39.6800	39.6800	0.0000	0.0000	-0.1000	0.1000
Distb_3 - Distb/Nominal,Xaxis (Cyl_3 - Cyl_5)						
Label	Nominal	Actual	Deviation	Lower Tol.	Upper Tol.	Oot
Diam	40.1000	40.1031	0.0031	0.0000	-0.1000	0.1000

4.2.1. Redesigning - Exhaust System Design Considerations

The waste heat areas of exhaust system were analysed by measuring the dimensions of connector, flanges and pipe. The existing exhaust system has a potential to accommodate waste heat recovery system in it. Hence, it becomes necessary to study exhaust system design considerations, material selection and their properties.

The exhaust manifold is experiencing thermal fatigue as the temperature of the exhaust gases rises and falls. Internal pressure is subjected to the pressure waves of the generated exhaust gases at specific times during the cycle. The exhaust manifold will crack as a result of this. The breakdown of the exhaust manifold is mostly caused by thermal and mechanical loads. (Xin, 2013b)

Exhaust gases should be evacuated smoothly from the piston chambers to the exhaust manifold to improve engine output at high speeds. With an internal pressure load, structural and thermal analysis is performed, and stresses and deflections are documented. Efforts are being made to optimise the design for the aforementioned circumstances. There is a lot of effort put into improving performance and losing weight. Automobile manufacturers are attempting to reach a goal in engine design that is as efficient as possible. (Xin, 2013a)

Exhaust manifolds gather exhaust gases from engine cylinders and release them into the atmosphere via the exhaust system. The combustion parameters of the engine would be determined by how the exhaust gases were evacuated from the cylinder. The following are some of the most important characteristics of exhaust manifold design for internal combustion engines. (Kanazaki et al., 2003)

1. The exhaust manifold should be designed to keep the exhaust pipe at a high temperature. This is required because a catalyst near the exhaust pipe's end would absorb more pollution in high-temperature settings.
2. To avoid any damage, the design should guarantee that the natural frequencies of the exhaust manifold are not within the excitation frequency range of engine vibration.
3. The exhaust manifold's mass should be as low as possible.

4.2.2. Material considerations for exhaust system

Exhaust systems are meant to meet regulatory standards by decreasing noise, vibrations, and harshness while managing emissions. The exhaust system includes the manifolds, closely linked and underbody catalytic converters, flexible bellow, muffler, resonator, connecting pipes, flanges, and tailpipe. The manifold, converter, and flex joint are all part of the hot end segment of the exhaust system. Because of the heated exhaust gas travelling through these components, this part of the system is relatively hot.

The component, which consists of an intermediate pipe, a resonator, and a muffler, is referred to as the cold end because the gas tends to cool as it exits the flex tube. The hot end of a gasoline-powered vehicle can reach temperatures of up to 1050°C, while the cold end can reach temperatures of up to 650°C. (McCune & Weber 2001) The material used in an exhaust system is determined by a number of factors, including the temperature at which it will be used, the geographical region in which it will be used, and the application.

Depending on the vehicle application, different materials are used. The most frequent materials used in exhaust systems are cast iron, stainless steel, and mild steel/carbon steel. Due to contemporary trends in light weight designs, cost reduction, and increased performance, designers are turning to sheet metals. Stainless steel is now used in flexible bellows, catalytic converters, resonators, mufflers, and pipes. Mild steel or carbon steel flanges, pipes, and mufflers are used.

In this research, a thermionic emission material having lower work-function is the primary consideration for any material selection. Whereas, the assembly of designed regenerator is supposed to be done in exhaust system, the material should satisfy the exhaust system design considerations also. It becomes necessary to study the behaviour of existing exhaust pipe materials as well as thermionic emission materials for the performance. Therefore existing materials and their properties are also considered which are taken in the further studies.

4.2.3. Existing Materials

From the above discussion existing exhaust pipe materials and their properties considered in this research work are shown in Table 4.3 and 4.4. The significance of each material is mentioned in description section.

Table 4.3. Materials Considered for Analysis (McCune & Weber, 2001)

Sr. No.	Material	Description
1	SS400	Carbon, silicon, manganese, and low quantities of phosphorus and sulphur make up SS400 steel. It's one of the most often utilised types of hot-rolled structural steel.
2	SUH409L	Grade 409L (UNS S40900, EN 1.4512) is a stable variant of 409, made up of the right amount of chromium, a low carbon and nitrogen content, and the addition of titanium. This combination of qualities gives Grade 409L its corrosion resistance, weldability, and formability.
3	SUS439L	Where temperatures tend to exceed the oxidation limit of grade 409 steel, stainless steel grade 439 can be formed into complex shapes such as tubular manifolds and exhaust system components. When moist corrosion resistance, particularly against chlorides, is required, it is also favoured. Weldability, brightness, and pitting corrosion resistance are all strengths of stainless steel grade 439. It polishes nicely and is suitable for detailed drawing.
4	SA1D	Aluminized steel is steel that has had an aluminum-silicon alloy hot-dip coated on both sides. This method ensures a strong metallurgical link between the steel sheet and the aluminium covering, resulting in a material with a unique set of qualities that neither steel nor aluminium alone can offer.

The criteria for material selection for exhaust system are; Thermal sustainability, Corrosion resistance, Vibration sustainability. In addition to this for thermionic conversion low work function of material is criteria. Therefore for this study existing exhaust pipe materials are also considered to compare their performance with thermionic emission materials like, tungsten & molybdenum.

Table 4.4. Thermal, Mechanical and Thermionic Emission Related Properties
(McCune & Weber, 2001)

Sr. No.	Material	Melting Point (°C)	Thermal Conductivity (W/mK)	Young's Modulus (GPa)	Work Function (eV)	Poisson's Ratio	Density (Kg/m ³)	Coefficient of thermal Expansion (x 10 ⁻⁶)
1	SS400	1430	16	210	4.4	0.26	7860	17.8
2	SUH409 L	1510	25	200	4.4	0.3	7750	11.7
3	SUS439 L	1505	14	193	4.4	0.29	7700	13
4	SA1D	677	15	200	4.4	0.24	7870	13

4.2.4. Reverse Engineered Full Scale TRS (Redesigning)

Considering the parameters and materials for designing any exhaust system parts as mentioned in sections 4.2.1, 4.2.2 and 4.2.3, a full scale thermionic regeneration system (TRS) is designed. The pipe and connector dimensions measured were benchmark for redesigning the pipe. In addition to that the design is modified as per the thermionic energy conversion requirements.

The existing single exhaust pipe is redesigned with two hollow pipes (named emitter and collector) assembly as shown in Fig 4.13. This redesign is done by considering same design calculations as that of conceptual design. Inter-electrode gap, thermal and electrical insulation were considered while designing the parts. The final part and assembly drawings are shown in Fig. 4.14. To Fig. 4.20;



Fig. 4.13. Design of a Thermionic Regeneration System

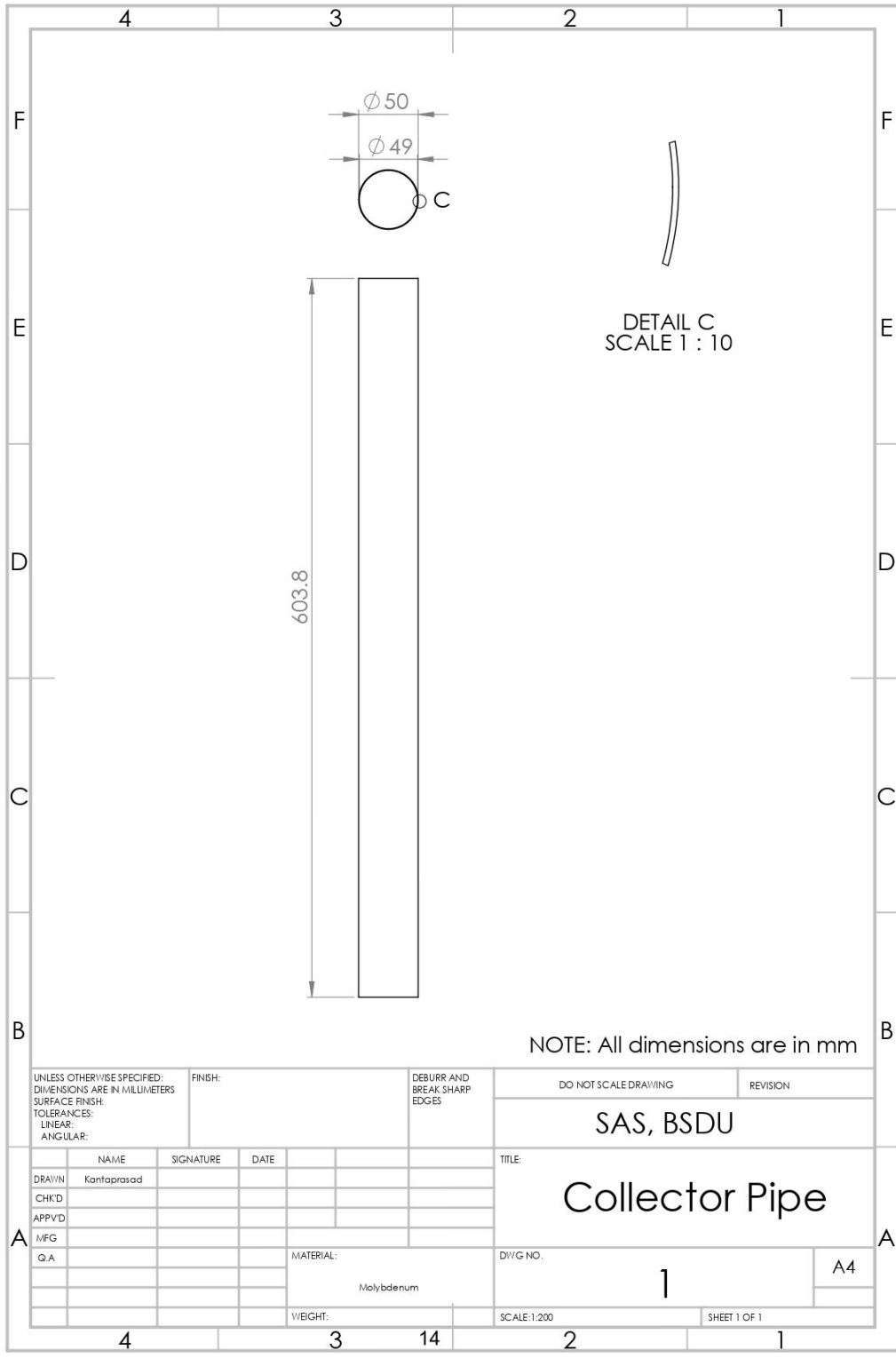


Fig. 4.14. Collector Pipe

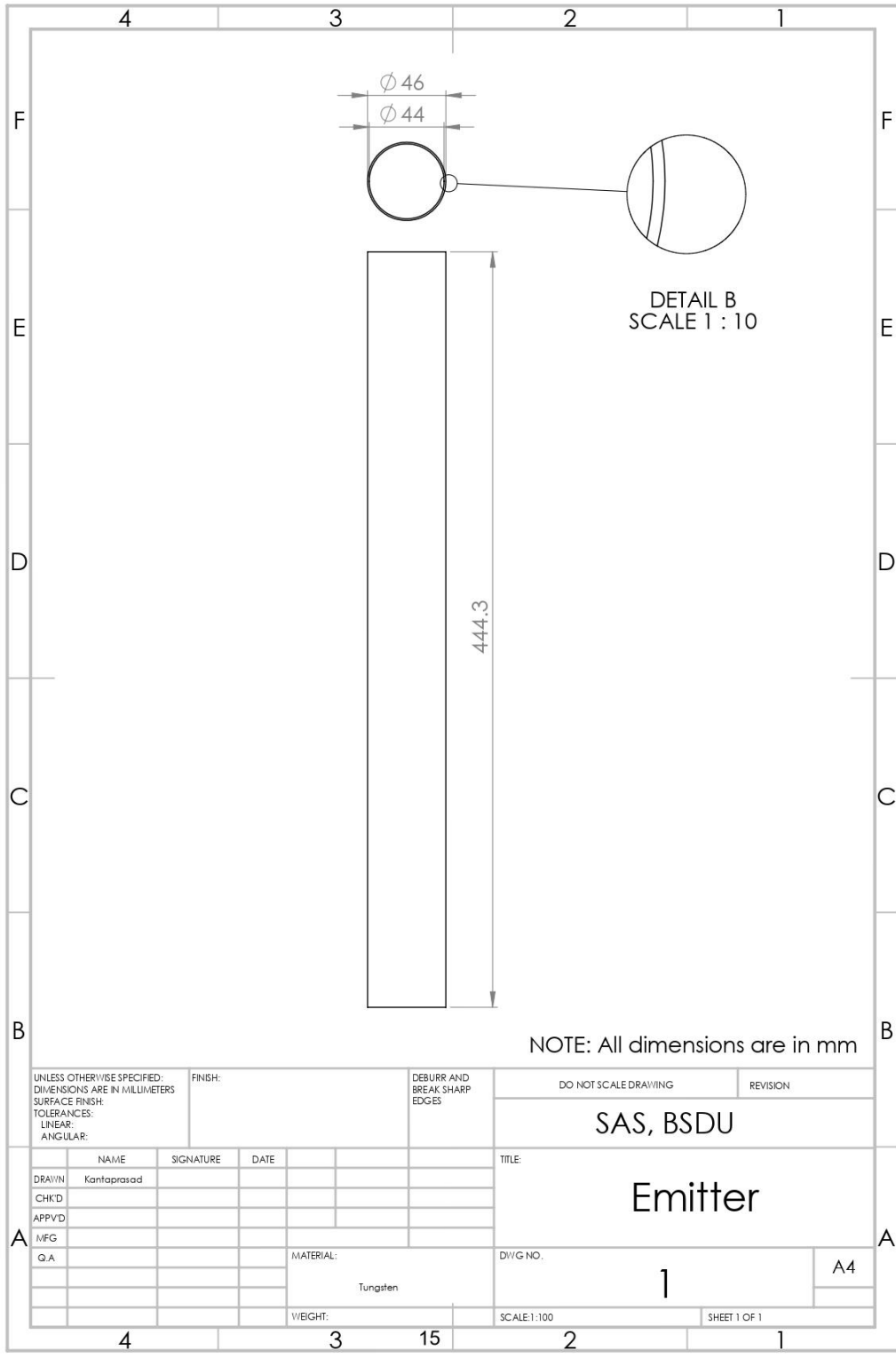


Fig. 4.15. Emitter Pipe

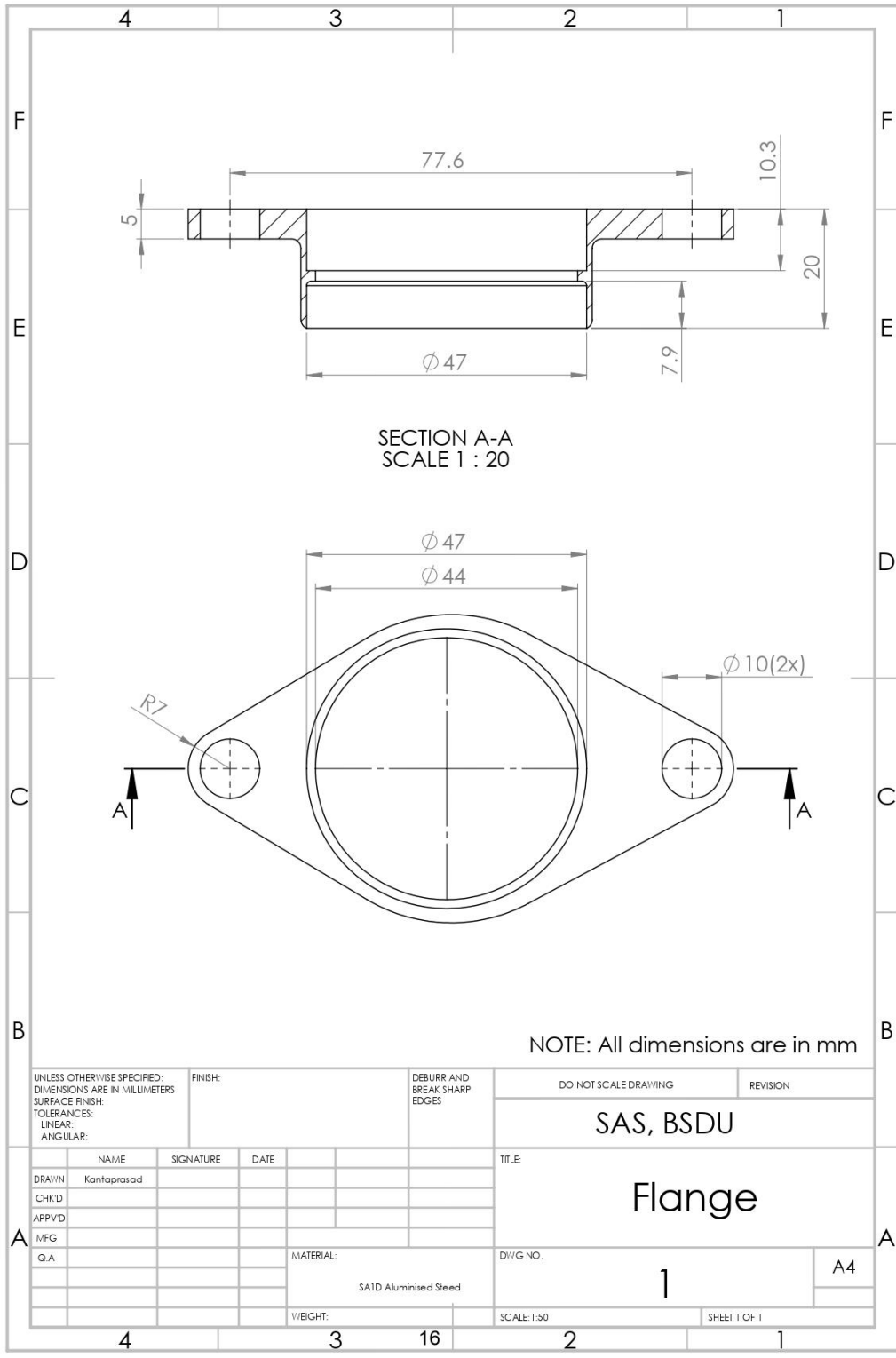


Fig. 4.16. Flange

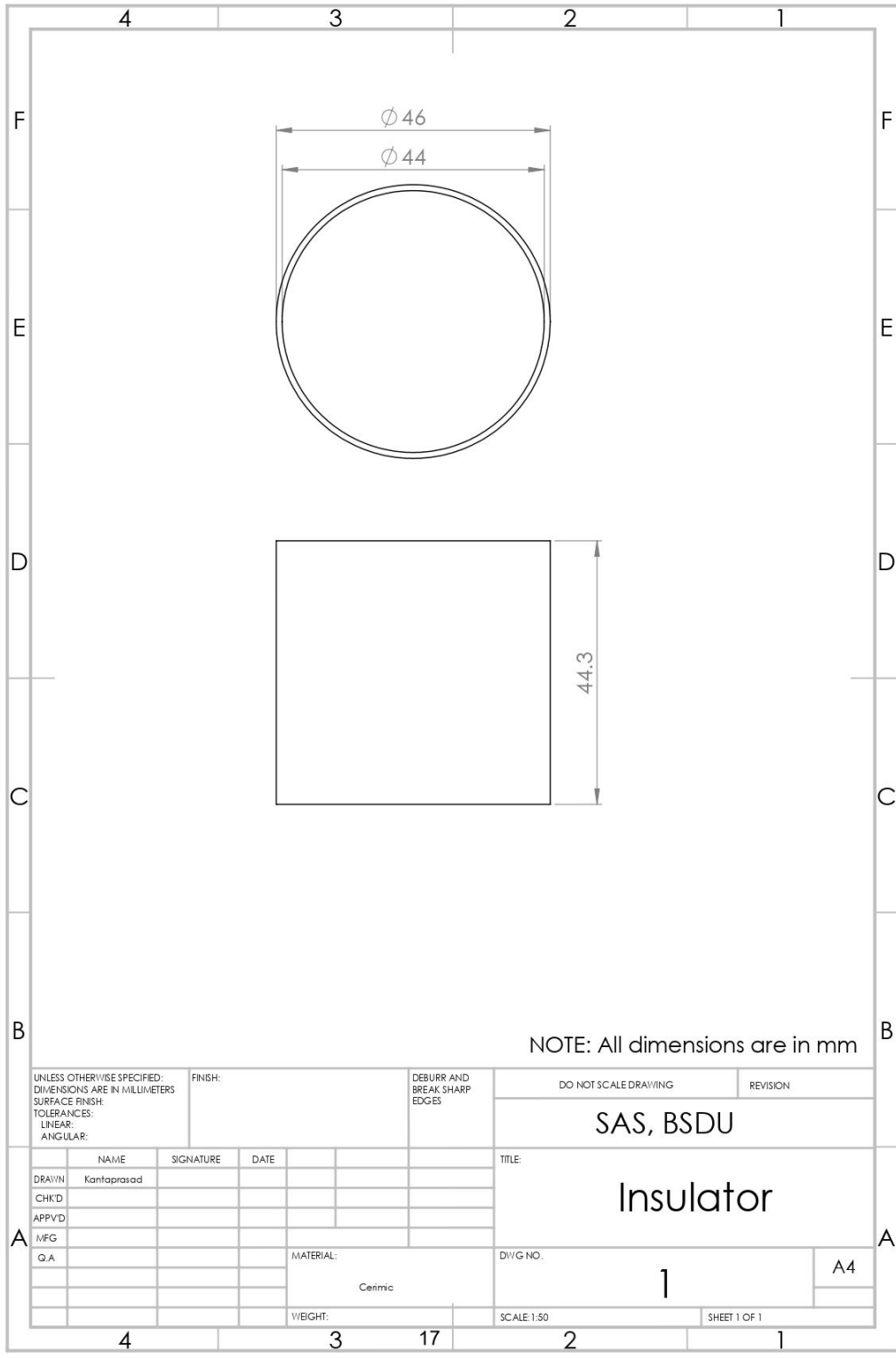


Fig. 4.17. Insulator

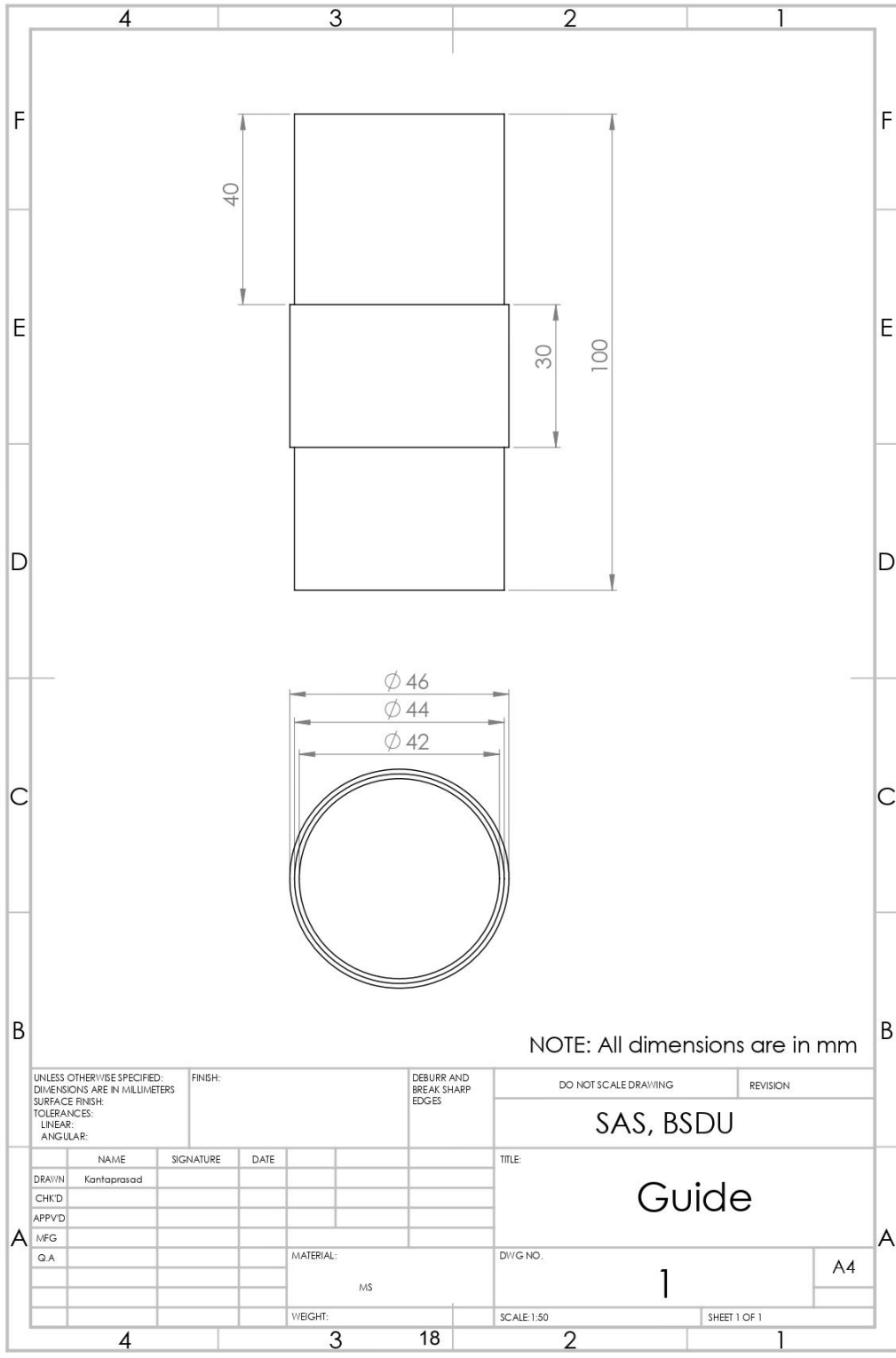


Fig. 4.18. Guide

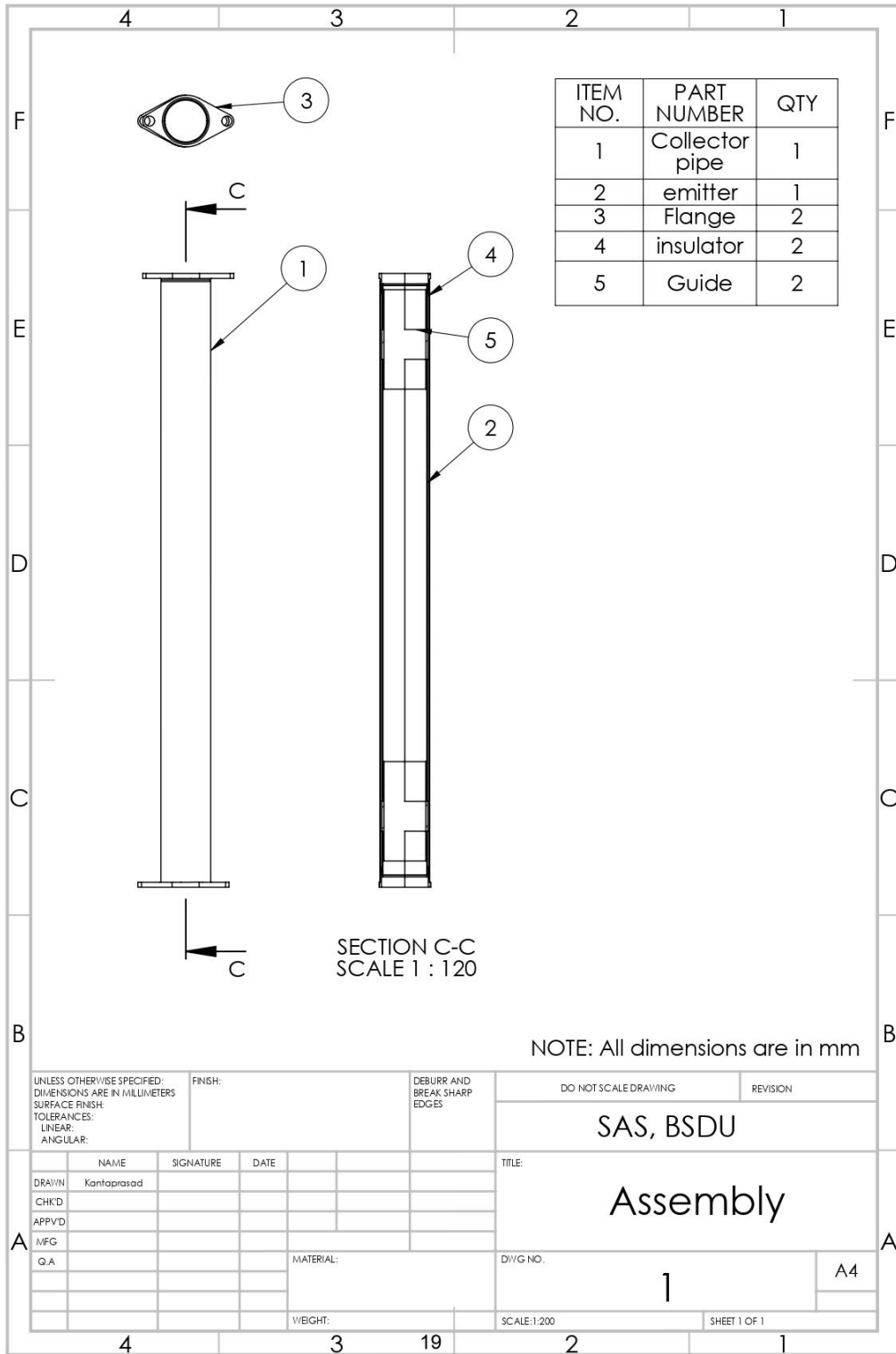


Fig. 4.19. Assembly

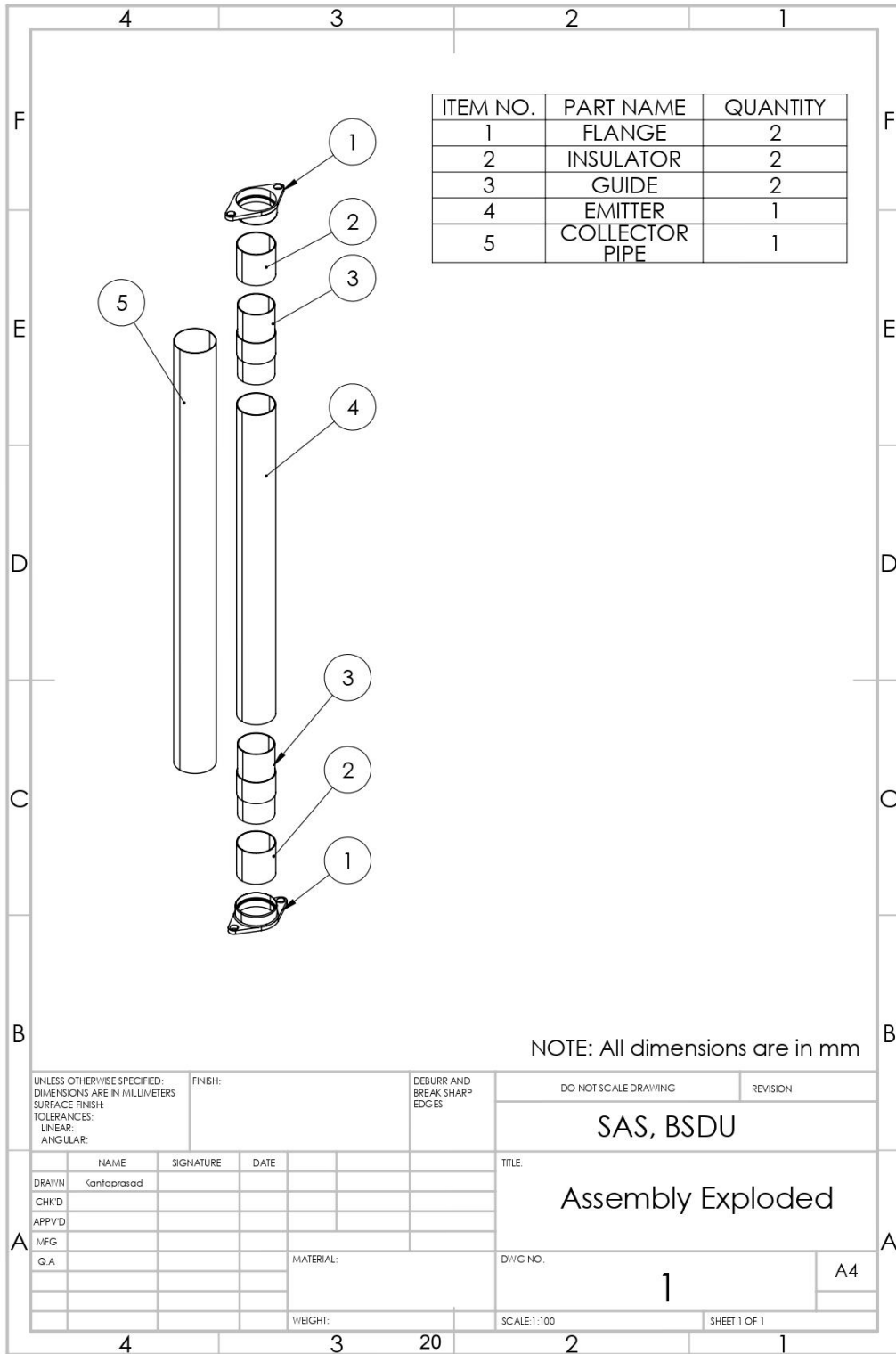


Fig. 4.20. Assembly Exploded

4.3 Analytical Study

Using the expression for thermionic emission, derived by Richardson and Dushman, the TEC fundamentals and technology were further modelled to simulate the performance. Comparing particle in cell model simulations with analytical model results have shown good agreement in terms of analysing space charge effect and modifying the converter design. Similar to this various software tools are available for modelling and simulating the TEC designs.

LabVIEW and COMSOL software are used in this work for developing an analytical study as well as design simulation. LabVIEW is a virtual interface software where mathematical expressions can be modelled. The designed test setup is modelled using a conceptual and analytical model for understanding the behaviour of thermionic regeneration system as explained below.(Kodihal & Sagar, 2019b)

4.3.1 Conceptual Model

A conceptual model from COMSOL multiphysics thermionic emission in a planer diode is considered here for the study. The model is shown in Fig. 4.20. This model is considered as a reference for studying thermionic regeneration from emission. The model description is as follows;

The thermionic regeneration system consists of two parallel electrodes separated by a distance $d = 0.5$ mm. The model geometry is three-dimensional but can be understood as quasi-1D because the potential and current are uniform in the x- and z-directions.

The geometry of the diode (as per the COMSOL model) and the functional form of the electric potential distribution in the space charge limited regime are illustrated in Fig. 4.21.

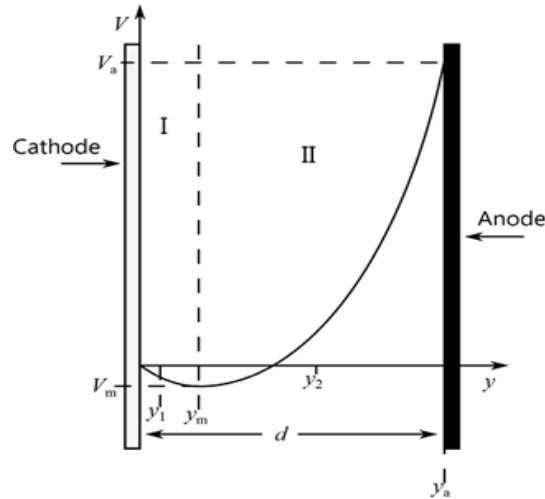


Fig. 4.21. Thermionic Regeneration System (*Models.Particle.Planar_diode.Pdf*, n.d.)

The cathode i.e. emitter is grounded V_c and the anode i.e. collector is maintained at a fixed potential of V_a . The cathode is maintained at a uniform temperature of T_c and its work function is Φ . Note that Figure 4.20 is not necessarily drawn to scale. The negative potential barrier is often extremely narrow compared to the diode width d .

The black solid curve shows the electric potential between the electrodes, which reaches a local minimum (V_m) at the potential barrier (y_m) before increasing closer to the anode. For computing the electric potential interpolation functions giving y_1 and y_2 as approximate function of y are displayed. y_1 and y_2 are corresponding values to y_m in region I and II respectively. The geometry is oriented so that the normal vector between the two parallel electrodes points in the positive y -direction. From the symmetry of the system, the transverse electric field components are zero ($E_x=E_z=0$), and the components of the electron velocity in these directions remain unchanged after they leave the cathode ($v_x = v_{x0}$, $v_z = v_{z0}$). This shows that the electron trajectories of y direction are significant for the study.

4.3.2. Analytical Model

The potential difference which can be obtained with the use of different materials as a thermionic emitter, is generally studied using Richardson Dushman equation and Child's Law. Power output and efficiency calculations for thermionic regeneration system are done by using mathematical expressions for heat to electricity conversion. Based upon this the following expressions are used to develop an analytical model for analysis.

Input Heat: The temperature of the emitter determines the emission of electrons, hence cathode heating is critical. As a result, the main three heating phenomena are regarded as input heat sources.

1) Electric Heating-

$$Q_{heat} = \frac{V^2}{R} \dots\dots\dots\text{Equation (1)}$$

Where,

V = Voltage

R = Resistance

OR

2) Exhaust Gas heat supply-

$$Q_{heat} = m_g C_{pg} (T_2 - T_1) \dots\dots\dots\text{Equation (2)}$$

Where,

m_g= mass flow rate of gas kg/min

C_{pg}= specific heat of gas KJ/Kg K

T₂= Input Temperature

T₁= Output Temperature

OR

3) Overall Heat transfer coefficient-

Thermionic generator has a cathode and anode construction where cathode gets heated and emits the electron in a closed inert gas environment. The Coefficient of heat transfer is needed to analyse the amount of heat transferred to the cathode with exhaust gas flow. This can be found by considering whole phenomenon as an Internal forced convection.

The flow of gas whether it is laminar or turbulent is given by Reynolds number.

Following expression is used for calculating Reynolds number

$$R_e = \frac{4m_g}{\pi D \mu} \dots\dots\text{Equation (3)}$$

Where,

M_g = mass flow rate of gas Kg/sec

μ = Viscosity Kg/m.sec

D = Outer diameter of Pipe

For turbulent flow, flow through pipe is given by;

A relation based on direct heat transfer measurements i.e.

$$Nu_d = 0.023Re_d^{0.8}Pr^n \quad \dots\text{Equation (4)}$$

(Dittus Boelter Equation)

Nu_d = Nusselt Number

Re_d = Reynoulds Number

Pr = Prandtle Number

$n=0.4$ for heating

$n=0.3$ for cooling

Heat transfer coefficient is given by,

$$h = \frac{Nu_d \times K}{D} \quad \dots\text{Equation (5)}$$

Where;

h = coefficient of heat transfer

K = Thermal Conductivity of Fluid

D = Diameter of Pipe

Power Output: Thermionic emission directly converts heat energy into electric energy.

The current density equation is used here.

1) Richardson Dushman's Equation for thermionic emission

$$J_{th} = AT^2 \exp \frac{-\phi}{k_B T} \quad \dots\text{Equation (6)}$$

Where,

J = Current Density A/mm²

T = Emitter Temperature

Φ = Emitter Work Function

A = Richardson Constant

K_B = Boltzmann's constant

2) Area of Emitter surface

$$A_e = 2\pi r h + 2\pi r^2 \quad \dots \text{Equation (7)}$$

r = radius of pipe

h = height/ length of pipe

3) Electric Potential and Power Output

$$P_{\text{output}} = V \times I \quad \dots \text{Equation (8)}$$

Where,

V = Voltage Output (V)

I = Current (A)

4.3.3 Efficiency of Thermionic Generator

$$\text{Conversion Efficiency} = \frac{\text{Electric power output}}{\text{Heat input}} \dots \text{Equation (9)}$$

Solved Example for Heat Transfer and Thermionic Conversion

Exhaust gas is flowing from a 1m long hollow cylindrical tungsten emitter with inner diameter of 51mm and outer diameter of 54mm at a rate of 0.056 kg/s and at pressure of 500 kPa. The temperature of pipe measured after the exhaust manifold is 800⁰C.

- i. Calculate the rate of heat transferred to the surface of emitter.
- ii. Find the thermionic emission from the emitter surface showing its current density.
- iii. Find the potential difference between tungsten emitter and molybdenum collector if the interelectrode gap kept is 0.5 mm.
- iv. What is the conversion efficiency of the system?

Given:

- 1) For flue gases viscosity at 800°C, $\mu = 4.362 \times 10^{-5}$
- 2) Mass flow rate of exhaust gas, $m_g = 0.056 \frac{kg}{sec}$
- 3) Prandtl number for give pressure and temperature, $Pr = 0.7149$ (*Appendix II: Prandtl Number chart*)
- 4) Dittus boelter equation constant, $n = 0.3$
- 5) Tungsten work function $\Phi_e = 4.5$ eV
- 6) Molybdenum work function $\Phi_c = 4.32$ eV
- 7) Richardson constant $A = 60$
- 8) Stefan–Boltzmann constant $K_B = (8.6173 \times 10^{-5})$
- 9) Child's Law Constant $K = 0.0023340$
- 10) Thermal Conductivity of Fluid $K_T = 0.07465$

Solution:

- Calculating Reynold's number for determining the flow,

$$\begin{aligned}
 Re &= \frac{4(0.056)}{\pi (0.021)(1.80 \times 10^{-5})} \\
 &= \frac{4(0.056)}{0.00000118884} \\
 &= 77874.03
 \end{aligned}$$

$Re > 4000$ i. e the flow is turbulent

- A relation based on direct heat transfer measurements. Using Dittus Boelter equation,

$$\begin{aligned}
 N_{ud} &= 0.023(77874)^{0.8}(0.7149)^{0.4} \\
 &= 292.40
 \end{aligned}$$

- Total Heat flux,

$$\begin{aligned}
 h &= \frac{292.40 \times 0.07465}{0.0255} \\
 \mathbf{h} &= \mathbf{1038.73 \frac{W}{m^2K}}
 \end{aligned}$$

- Surface area of emitter,

$$\begin{aligned}
 A_e &= 2\pi rh + 2\pi r^2 \\
 A_e &= 2\pi(25.5)(1000) + 2\pi(25.5)^2 \\
 A_e &= 164.30 \times 10^3 \text{ mm}^2 = 0.164 \text{ m}^2
 \end{aligned}$$

- Current density through thermionic emission,

$$\begin{aligned}
 J_{th} &= AT^2 \exp \frac{-\Phi}{k_B T} \\
 J_{th} &= 60(1073.15)^2 \exp \frac{-(4.5)}{(8.6173 \times 10^{-5})1073.15} \\
 J_{th} &= 43.86 \frac{\text{A}}{\text{m}^2}
 \end{aligned}$$

- Minimum Electric potential,

$$\begin{aligned}
 J &= \frac{KV_d^{\frac{3}{2}}}{d^2} \\
 V_d &= \frac{d^2 J^{\frac{2}{3}}}{K} \\
 V_d &= \frac{(0.5)^2 (43.86)^{\frac{2}{3}}}{0.0023340} \\
 &= 3.495 \text{ V}
 \end{aligned}$$

- Total Electrical power output

$$\begin{aligned}
 E_{output} &= V \times I \\
 &= 3.4 \times (43.86 \times 0.16) \\
 &= \mathbf{23.86 \text{ W}}
 \end{aligned}$$

- Conversion Efficiency,

Conversion Efficiency

$$= \frac{\text{Electric power output}}{\text{Heat input}}$$

$$\eta = \frac{\text{Electric power output}}{\text{Heat input}}$$

$$\eta = \frac{23.86}{166.08} = \mathbf{14.3\%}$$

The same example is solved by considering 100 microns graphene coating on emitter external surface and collector inner surface with a work functions of 1.1 eV and 1.0 eV respectively.

Solution:

- Calculating Reynold's number for determining the flow,

$$\begin{aligned} Re &= \frac{4(0.056)}{\pi (0.021)(1.80 \times 10^{-5})} \\ &= \frac{4(0.056)}{0.00000118884} \\ &= 77874.03 \end{aligned}$$

$Re > 4000$ i.e the flow is turbulent

- A relation based on direct heat transfer measurements. Using Dittus Boelter equation,

$$\begin{aligned} N_{ud} &= 0.023(77874)^{0.8}(0.7149)^{0.4} \\ &= 292.40 \end{aligned}$$

- Total Heat flux,

$$\begin{aligned} h &= \frac{292.40 \times 0.18447}{0.0256} \\ \mathbf{h} &= \mathbf{2107.09 \frac{W}{m^2K}} \end{aligned}$$

- Surface area of emitter,

$$\begin{aligned} A_e &= 2\pi rh + 2\pi r^2 \\ A_e &= 2\pi(25.6)(1000) + 2\pi(25.6)^2 \\ A_e &= 164.96 \times 10^3 \text{ mm}^2 = 0.16496 \text{ m}^2 \end{aligned}$$

- Current density through thermionic emission,

$$\begin{aligned} J_{th} &= AT^2 \exp \frac{-\Phi}{k_B T} \\ J_{th} &= 60(1073.15)^2 \exp \frac{-(1.1)}{(8.6173 \times 10^{-5})1073.15} \\ J_{th} &= 17.1096 \frac{A}{m^2} \end{aligned}$$

- Minimum Electric potential,

$$J = \frac{KV_d^{\frac{3}{2}}}{d^2}$$

$$V_d = \frac{d^2 J^{\frac{2}{3}}}{K}$$

$$V_d = \frac{(0.3)^2 (17.1096)^{\frac{2}{3}}}{0.0023340}$$

$$= 16 \text{ V}$$

- Total Electrical power output

$$E_{output} = V \times I$$

$$= 16 \times (17.1096 \times 0.16)$$

$$= \mathbf{43.8 \text{ W}}$$

- Conversion Efficiency,

Conversion Efficiency

$$= \frac{\text{Electric power output}}{\text{Heat input}}$$

$$\eta = \frac{\text{Electric power output}}{\text{Heat input}}$$

$$\eta = \frac{43.8}{166.08} = \mathbf{26.37\%}$$

The above equations were used to develop a simple LabVIEW module to analyze the heat transfer and thermionic conversion efficiency at variable emitter temperatures and materials. The modules are shown in Fig. 4.21 and 4.22.

The software has two windows named front panel and block diagram. These windows help us to create model using expressions and tools.

Front Panel: Fig. 4.22 shows a front panel developed for thermionic energy conversion representation. Front panel has indicators and displays like thermometer, control knob, switch etc. Various electromechanical tools are available on front panel representing the actual setup.

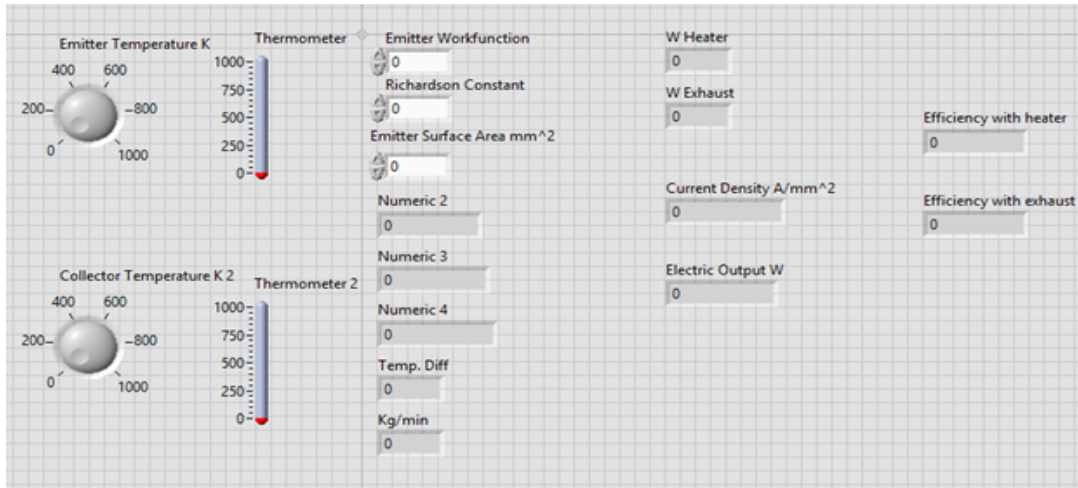


Fig. 4.22. Front Panel (Courtesy: LabVIEW)

Block diagram: Fig. 4.23 shows the representation of mathematical expressions discussed above. The above equation are framed in combination to present a mathematical model for calculating thermionic energy conversion efficiency. Block diagram is a flow of numerical calculations using numerical tools in the window. It has functions pallet to select the expression and a tool pallet to connect the expressions. The block diagram once modelled, replicates in the front panel. This combined model is divided into three parts.

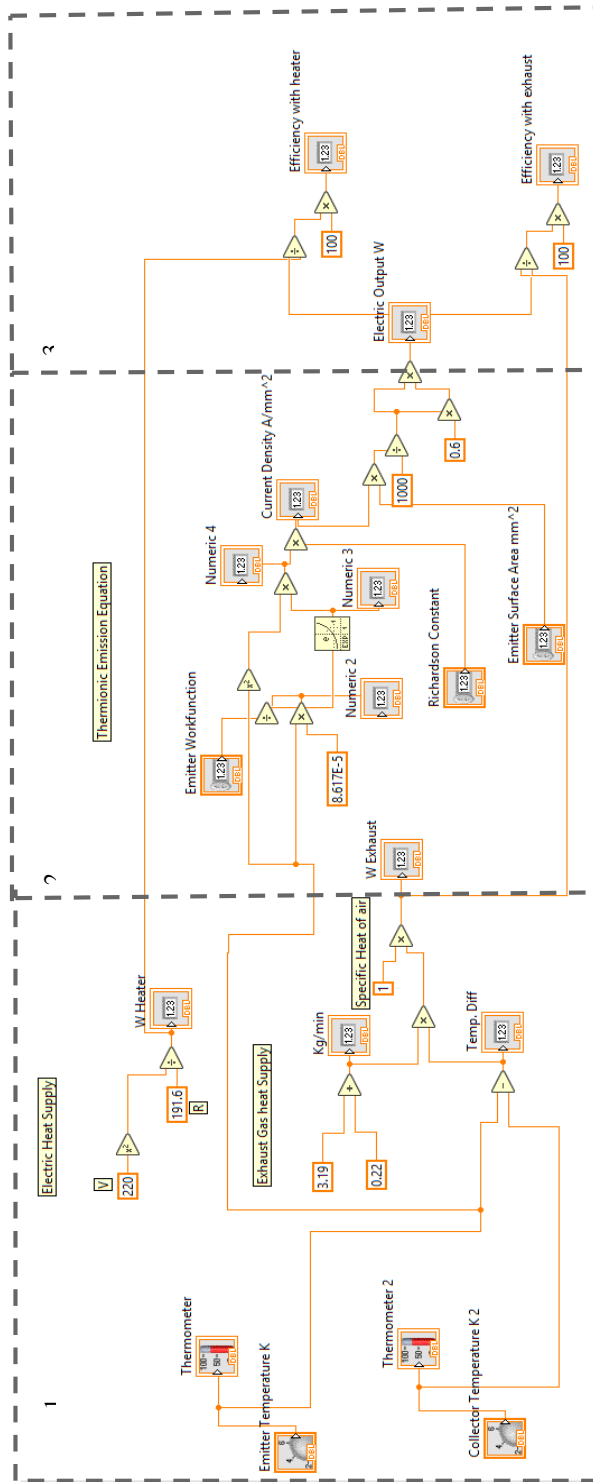


Fig. 4.23. Block Diagram (Courtesy: LabVIEW)

The block diagram in Figure 4.23 is divided into three sections. Input heat, thermionic emission & out efficiency equations.

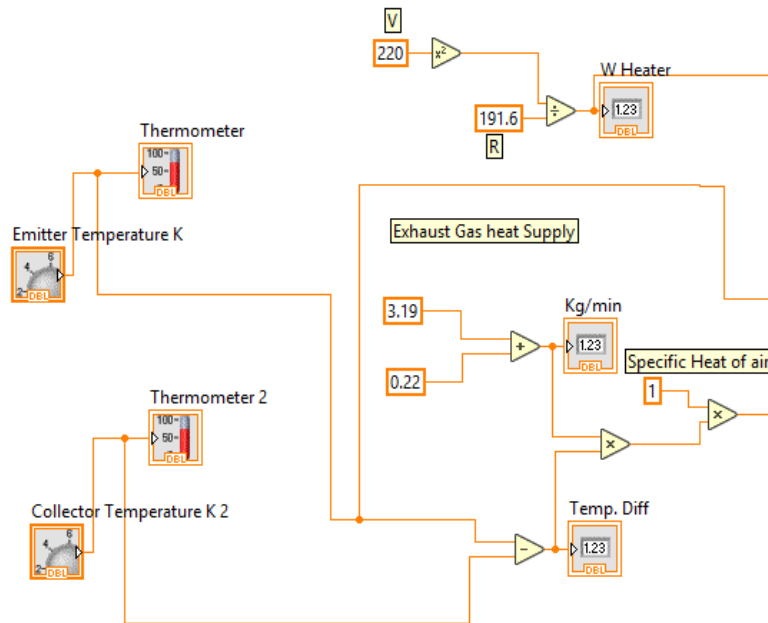


Fig. 4.24. Input Heat Equations on Block Diagram (Courtesy: LabVIEW)

Section 1: Input heat equations (1) & (2) are modelled as shown in Fig 4.24. Exhaust gas heat is calculated with mass flow rate of gas, temperature difference and specific heat of exhaust air. Two control knobs are used to set the temperatures of emitter and collector.

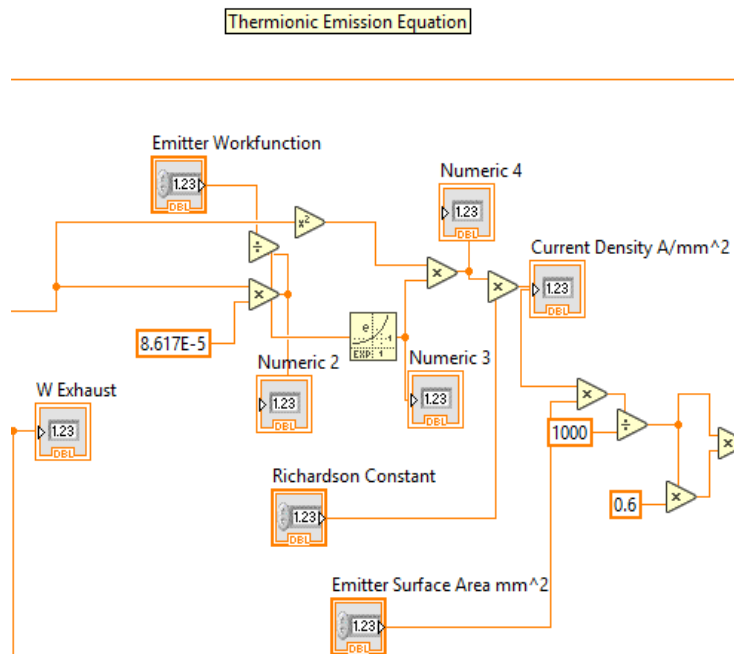


Fig. 4.25. Thermionic Emission Equation on Block Diagram (Courtesy: LabVIEW)

Section 2: Equations (3), (4), (5), & (6) are modelled as shown in 2nd section above. This block diagram has thermionic emission equations which calculate the current density and potential difference achieved from conversion.

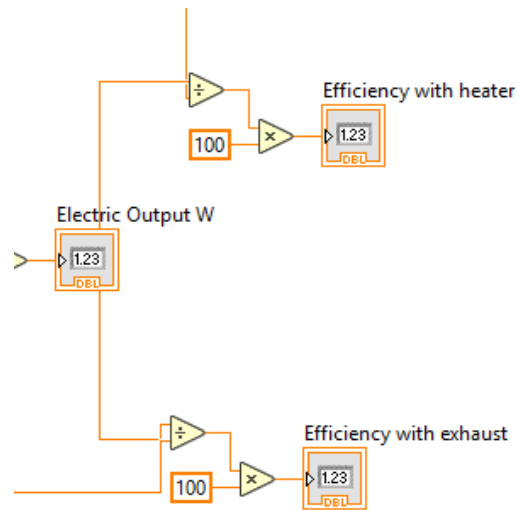


Fig. 4.26. Output and Efficiency Equation on Block Diagram (Courtesy: LabVIEW)

Section 3: The block diagram in Fig. 4.26 uses equations (7), (8) & (9) for calculating overall efficiency of a thermionic energy conversion system.

4.4. Design, Modelling and Simulations

This solid works design is simulated on COMSOL multiphysics Software using Thermionic Emission model. This is a benchmark model for analysing the effect of space charge. Charged particle tracing interface is used to model the thermionic emission through the hot emitter surface. (*Models.Particle.Planar_diode.Pdf*, n.d.) The transmitted current and the potential is compared with the analytical solution of Langmuir-Fry model. The geometry is imported from the SolidWorks as shown below;

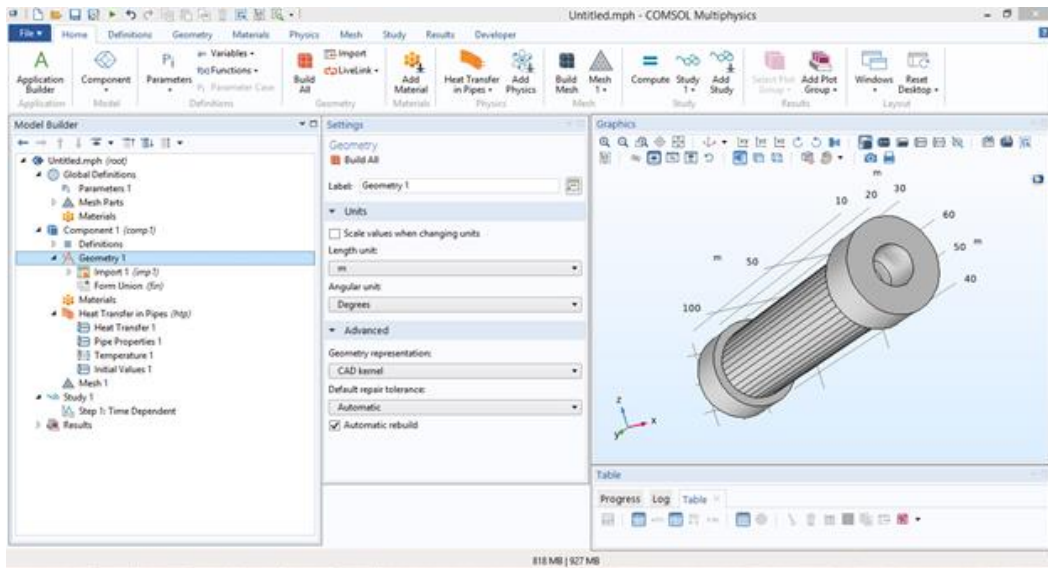


Fig. 4.27. COMSOL Work Window (Courtesy: COMSOL Multiphysics)

The work window shown in Figure 4.27 can be divided into three panels;

- 1) Model Builder
- 2) Settings
- 3) Graphics

1) Model Builder: This window features the input parameters like selecting the geometry, material, multiphysics study and result. The window shown in Fig. 4.28 is for prototype design model building including physics options.

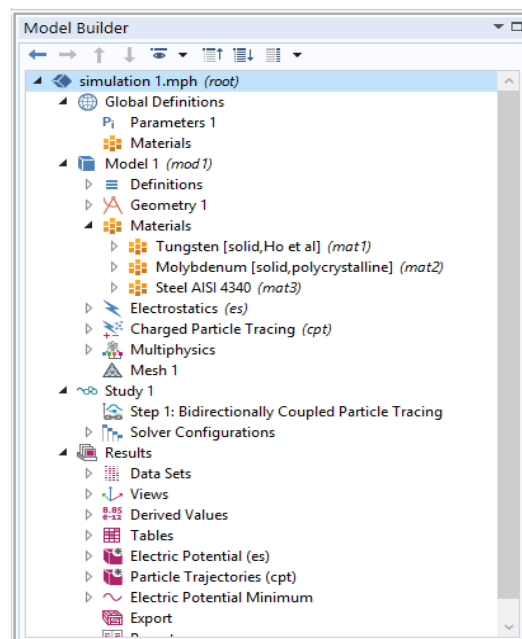


Fig. 4.28. Model Builder (Courtesy: COMSOL Multiphysics)

Simulation Modes: Electrostatics, charged particle tracing and multiphysics;

Considering its automotive application the cathode i.e. Emitter gets heated due to the hot gas flowing through it. Whereas the test setup is designed to heat the emitter by electric cartridge heater. Therefore for the simulation of temperature profile of an emitter and collector a convective heat transfer is considered. The temperature gradient is assumed to be 500⁰C.

The charged particle tracing model evaluates the current density of the device at specified emitter temperature. Multiphysics combines both physics interface and simulates the design accordingly. The values for thermionic emission are taken from material and the study uses bidirectionally coupled particle tracing.

2) Settings: The model input specified in model builder can be edited with dimension, unit, equation, design etc. using settings tab, as shown in Fig 4.29.

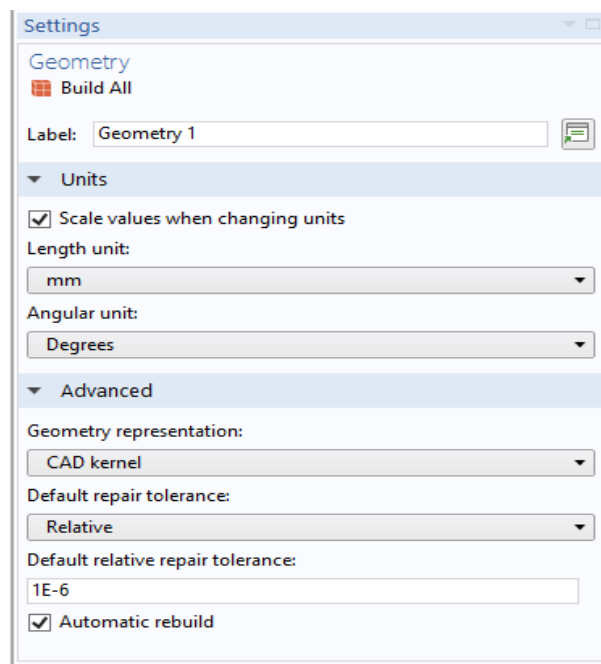


Fig. 4.29. Settings (*Courtesy: COMSOL Multiphysics*)

3) Graphics: It is a 2D and 3D design workplace where design can be imported, modified or created. The modelled thermionic emission can be simulated with the graphics design as shown in Fig 4.30.

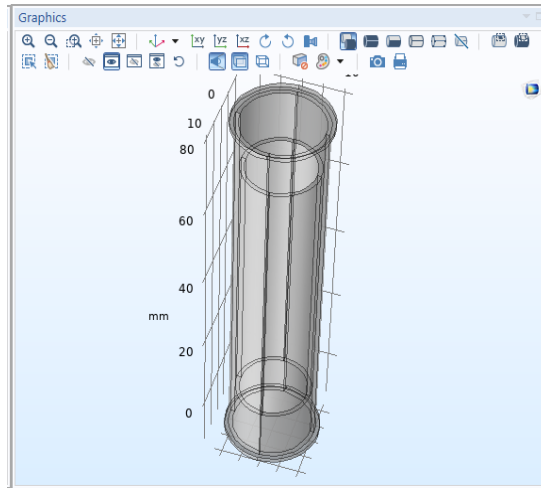


Fig. 4.30. Graphics (Courtesy: COMSOL Multiphysics)

4.5. Heat Transfer and Thermionic Conversion Analysis

The performance of a designed thermionic regeneration system is analysed by mathematical calculations for heat transfer, thermionic energy conversion. Thermionic generator has a cathode and anode construction where cathode gets heated and emits the electron in a closed inert gas/vacuum environment. The rate of heat transfer is needed to analyse the amount of heat transferred to the cathode with exhaust gas flow. This can be found by considering the phenomenon as an Internal forced convection through pipe. This analysis is done through mathematical equations of heat transfer from gas to the emitter surface.

4.5.1. Thermionic Conversion Analysis

Thermionic emission from the surface is analysed through Richardson-Dushman equation and potential difference between emitter and collector through Child's Law previously for prototype test setup. Same mathematical expressions are used for thermionic conversion analysis of a designed large scale thermionic regeneration system shown in figure. The design is then simulated using thermionic emission module of COMSOL multiphysics software.

$$J_{th} = AT^2 \exp \frac{-\phi}{k_B T} \dots \text{Richardson-Dushman Equation (4)}$$

J_{th} = Emission Current Density in amp/m²

T = Surface Temperature in Kelvin

A = Plank Constant

$-\Phi$ = work function of the material

K_B = Boltzmann constant

$$J = \frac{KVd^{\frac{3}{2}}}{d^2} \dots \text{Child's Law (5)}$$

V_d = Potential difference between emitter and collector

d = diameter of the pipe

K = Child's law constant

The block diagrams in Fig 4.31 & 4.32 are developed using expressions of heat transfer and thermionic conversion explained in early chapter.

4.5.2 LabVIEW Modules

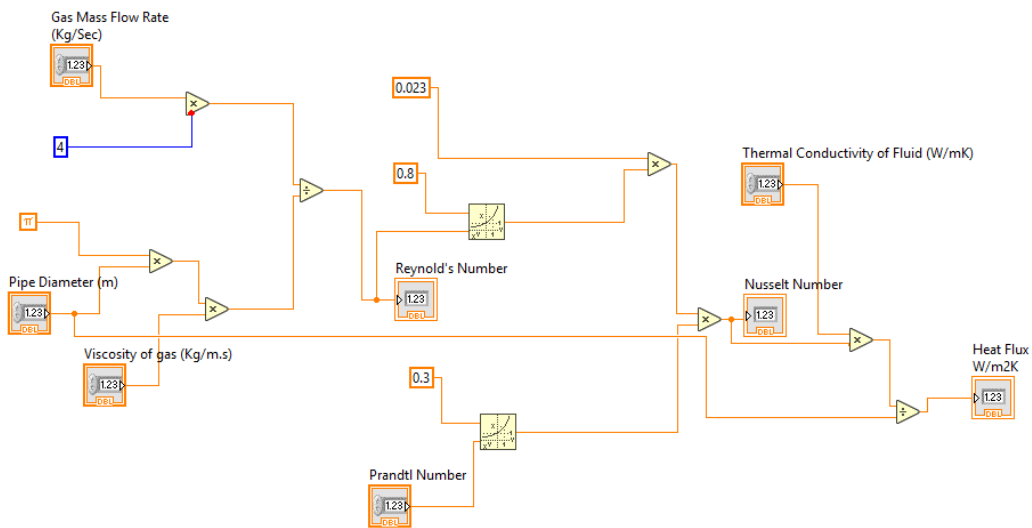


Fig. 4.31. Heat Transfer Analysis on LabVIEW (Courtesy: LabVIEW)

This block diagram shown in Fig 4.31. Represents mathematical expression for amount of heat transferred from exhaust gases to the surface of the exhaust pipe.

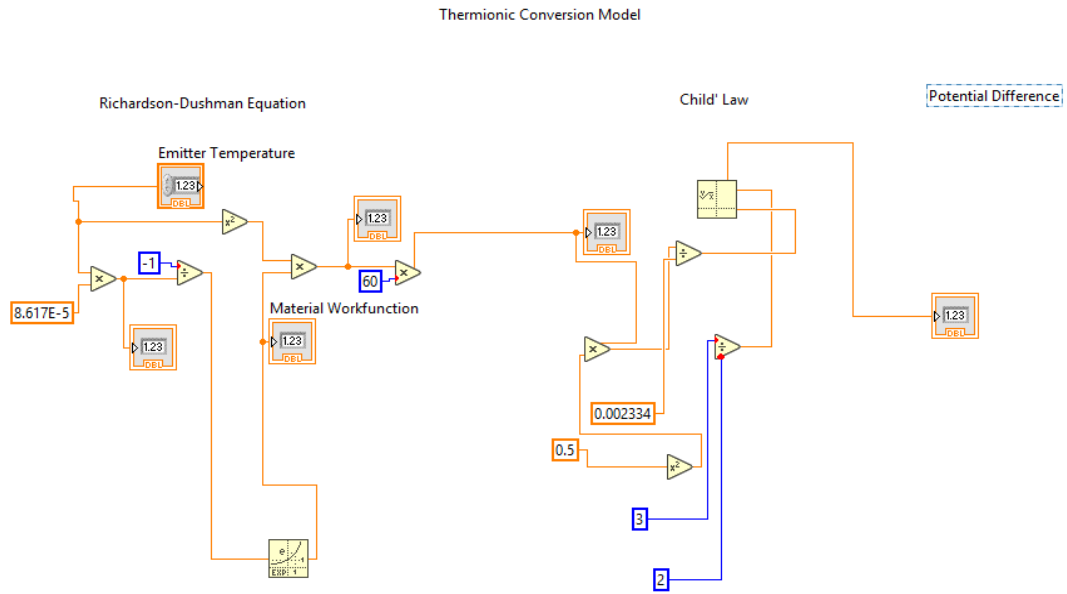


Fig. 4.32. Thermionic Conversion Analysis on LabVIEW (Courtesy: LabVIEW)

This block diagram shown in Fig 4.32. Represents mathematical expression for amount energy converted to electricity from the exhaust heat using thermionic emission.

4.5.3 Design Simulation

Process of Design Simulation for Thermionic Conversion

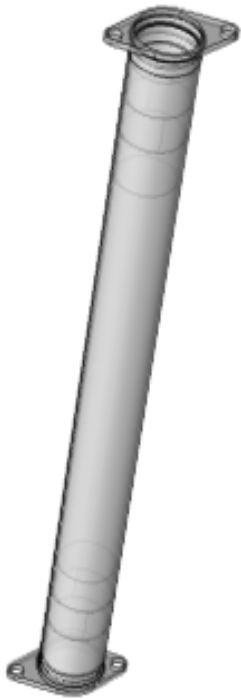


Fig. 4.33. Geometry Import

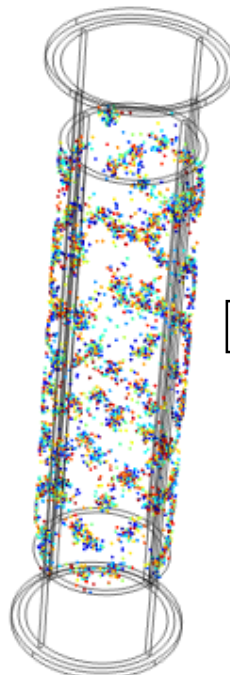
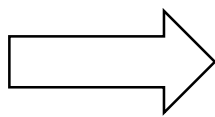


Fig. 4.34. Particle Trajectories
(Courtesy: COMSOL Multiphysics)

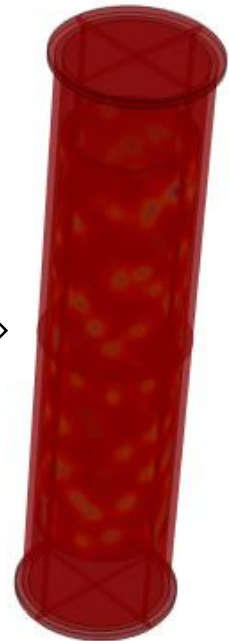
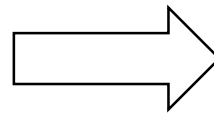


Fig. 4.35. Electric Potential

The design simulation is performed to study & compare the power output of a designed thermionic regenerator for selected emitter and collector materials. This is done by studying an existing module of “Thermionic Emission through Planer Diode is Comsol Multiphysics software. In this process a 3D design is simulated for thermionic emission. The emitter surface & collector surface are selected as boundary conditions and a ground electrode is needed to be finalised. The following steps are performed in the simulation.

1. The designed system is imported in COMSOL multiphysics software as shown in Fig. 4.33. (*Models.Particle.Planar_diode.Pdf*, n.d.)
2. Emitter and collector materials are selected from the Table 4.1 & 4.4.
3. Physics module of Electrostatics and Charged Particle tracing are selected.
4. Boundary conditions for Electrostatics and Charged Particle tracing are;
 - Heat transfer between emitter outer surface collector inner surfaces.
 - Collector is selected as an electrical ground.
5. Geometric mesh is generated using physics controlled fine mesh. The selected mesh is triangular prisms fine mesh.
6. Results for electric potential and particle trajectory are plotted as shown in Fig. 4.34 & Fig. 4.35. Graph for minimum electric potential between electrodes is plotted & discussed in results section.

4.6. Thermal Stress and Strain Analysis

The exhaust pipe is continuously under thermal load. The temperature of pipe varies from room temperature to max 800⁰C as mentioned in section 3.1.2. This leads to develop thermal stresses in the pipe. Therefore it becomes important to analyse the thermal stress developed and to improve the durability of a system. The thermal stress calculations are done by using mathematical equation shown below;

$$\sigma = E\alpha(T_f - T_o)$$

$$\sigma = E\alpha\Delta T \dots \text{Equation (6)}$$

$$\epsilon = A\sigma^n f_2(T) \dots \text{Equation (7)}$$

$$f_2(T) = e^{\frac{-12500}{T}} \dots \text{Equation (8)}$$

Where;

E = Young's modulus

α = coefficient of linear thermal expansion

A = stress normalization factor i.e. $3.0 \times 10^{-6}/h$,

T_f = maximum temperature in K,

T_o = Room temperature in K

σ = Thermal stress in MPa

n = the stress component

Solved Example:

Find the thermal stress and strain developed in an exhaust pipe made of tungsten, operating at 800°C . The volumetric coefficient of thermal expansion of tungsten is 4.3.

Given Data:

E = 700 GPa, $\alpha = 4.3$, $T_f = 800^\circ\text{C}$, $T_o = 30^\circ\text{C}$, n=5.5 (Stress Exponent)

$$\sigma = (700 \times 10^3)(4.3 \times 10^{-9})(800 - 30)$$

$$\sigma = \mathbf{2.31 \text{ MPa}}$$

$$\epsilon = (3 \times 10^{-6})(2.31)^{5.5} \left(e^{\frac{-12500}{1073}} \right)$$

$$\epsilon = \mathbf{0.0083}$$

The above equations are used to develop a LabVIEW module as shown in Fig 4.36 to perform numerical calculations by changing temperature and material properties for thermal stress and strain. The thermal stress strain analysis is done to understand the effect of thermal stress on Thermionic regeneration system.

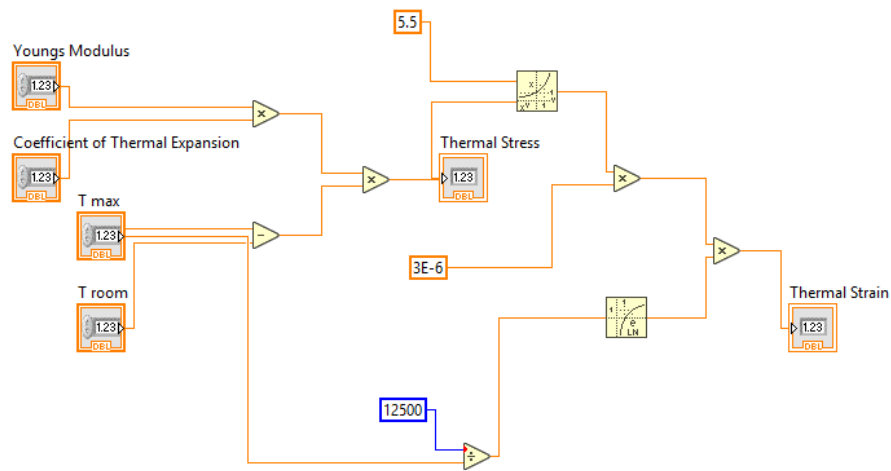


Fig. 4.36. Thermal Stress and Strain Equation (Courtesy: LabVIEW)

Design Simulation:

The Fig. 4.37, Fig. 4.38 & Fig. 4.39 shows the process of design simulation for thermal stress & strain using thermally induced creep module from Comsol Multiphysics software. This model computes the stress over a time of 10^{10} hour. All selected materials as emitter exhibits creep behaviour during heating.

Geometry: The geometry is a hollow cylinder with an outer diameter of 54 mm and an inner diameter of 51 mm. The problem is axisymmetric. In order to follow the original example, a rectangular sector (2D Model) is modelled.

Loads:

- An internal pressure of 500 kPa is applied. (The maximum exhaust gas pressure is 500kPa) (Xin, 2013b)
- The load will grow from zero to its full value in the first 0.1 seconds of the analysis.
- A temperature field with the distribution $T=333(1+100/r)$, this expression is used to distribute the temperature over the selected rectangle geometry.
- The boundary condition for this simulation is initiation of thermal load.
- The boundary layer selected for simulation of force distribution is shown in figure 4.36.

Process of Design Simulation for Thermally Induced Stress

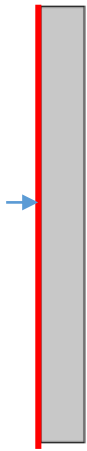


Fig. 4.37. 2D Axisymmetric Geometry with boundary load

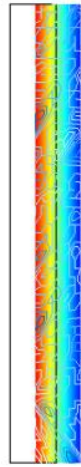
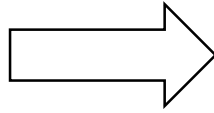


Fig. 4.38. Thermal stress strain analysis
(Courtesy: COMSOL Multiphysics)

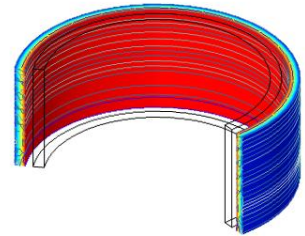
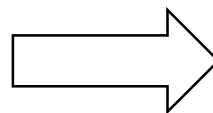


Fig. 4.39. 3D thermal stress strain analysis