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1	Theoretical and experimental evaluation of thermal interface materials and
2	other influencing parameters for thermoelectric generator system
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#### 13 Abstract

Thermal interface resistance of Thermoelectric Generator (TEG) plays a vital role in power 14 production. Improving surface finish of contact surfaces, applying pressure between the contact 15 16 surfaces and use of Thermal Interface Material (TIM) are few methods of reducing thermal resistance and thereby improving the efficiency of TEG. There is a need to evaluate the influence 17 of these methods and use them optimally for TEG system. Experiments were carried out to study 18 the influence of parameters such as thermal conductivity of TIM, contact pressure, surface 19 20 roughness and heat source temperature on the voltage and power outputs from TEG. Experimental results are validated with simulations using mathematical heat transfer model and COMSOLTM 21 22 Multiphysics numerical model. Appreciable agreement is seen between the experimental observations and model outputs. Experimental and model results indicate 0.6 W/mK as optimum 23 thermal conductivity for TIM material. Hence, use of costly TIMs like MWCNT (Multi Wall 24 Carbon Nano Tube) and copper nanoparticles may not be required for the selected application. 25 The contact pressure and surface roughness have appreciable influence when air is used as TIM. 26 These factors have insignificant influence for TIMs with higher thermal conductivity. Increase in 27 heat source temperature increases voltage and power output of TEG. 28

*Keywords*: Thermal Interface Material, Thermoelectric Generator, Heat Transfer Model,
COMSOL, Contact Pressure.

31 1. Introduction

Thermoelectricity, discovered in the 18<sup>th</sup> century, based on the principle of Seebeck effect, 32 promoted the development of thermoelectric generator (TEG). Currently, the acceptability of the 33 TEG is limited by its high capital cost and low energy conversion efficiency. Development of 34 material science and emerging ideas since the 1990s, focused on improving the figure of merit 35 (the ratio of the product of square of Seebeck coefficient, electrical conductivity and the 36 operational temperature to the thermal conductivity) of TEG materials, which revived the hope 37 for TEG to perform at par with the conventional heat engines. Recent advances have been reported 38 in Nanoscale thermoelectric materials [1-3], doping methodology [4-6], organic thermoelectric 39 materials [7], and oxide thermoelectric materials [8,9]. Commercially available TEG modules can 40 achieve a maximum efficiency of 7% [10], which could reach 15% at a figure of merit of 41 approximately 1.5 [11]. An availability of huge quantity of low temperature (< 200 °C) waste heat 42 in several industries [12-14], will only be fortuitous if a TEG system is developed to exploit this 43 low temperature waste heat. The potential of TEG system in conjunction with solar energy 44 technologies is also reported [15, 16] in literature. 45

Thermal Interface Material (TIM) is critical to achieve a higher conversion efficiency in the TEG 46 system. For obtaining maximum power, the thermal conductance of TIM interfaces with the heat 47 source and sink has to be maximised, which will also allow the exploitation of lower temperature 48 differences between two thermal contact surfaces. The TIM comprising of Carbon Nano Tube 49 (CNT) [17-19] is a potential candidate. An ideal TIM would eliminate the air gap, resulting in 50 51 zero temperature difference between the two contacting surfaces. This is not practically achievable, even though many studies have assumed so [20]. Astrain et al. [21] reported that a 52 10% decrease in thermal resistance can increase the power generated by up to 8%. Wang et al. 53 [22] experimentally investigated and analysed the effects of the interface material and loading 54 pressure factors on the thermal contact resistance and the performance of TEG. 55

Literature review indicates that no comprehensive study has been performed to evaluate and characterise the combined effects of contact pressure, surface roughness and thermal conductivity of TIM under varying heat source temperatures. Therefore, the objective of this paper is to optimize the thermal system for TEG applications by evaluating the effects of the aforementioned factors through a combined computer modelling and experimental programme. COMSOL<sup>TM</sup> Multiphysics has been employed for computer simulations and the model and simulation results have been validated against experimental results.

63

#### 64 2. Experimentation

Experiments under varying conditions were conducted and the open circuit voltage and closed 65 circuit power were measured. A schematic diagram of the experimental TEG set-up and its 3-D 66 view are shown in Fig. 1(a) and Fig. 1(b) respectively. The experimental set-up used for the 67 performance evaluation of TIM for TEG system is shown in Fig. 2. An electric heater was placed 68 between a steel holding plate and an aluminium heat spreader plate to simulate the heat source. A 69 70 K-type thermocouple of 1.5 mm diameter was placed in between the bottom of heat spreader plate and the electric heater to measure the heat source temperature (T<sub>hs</sub>) which was maintained by a 71 temperature controller through an electric resistance. Three TEGs were sandwiched between the 72 aluminium heat spreader plate (heat source side) and an aluminium fin heat sink. K-type 73 thermocouples were employed to measure heat spreader plate temperatures, T<sub>h1</sub>, T<sub>h2</sub> and T<sub>h3</sub> and 74 aluminium fin base plate temperature, T<sub>c1</sub>, T<sub>c2</sub> and T<sub>c3</sub>. The contact area between the TEG and 75 aluminium heat spreader plate on hot side and between TEG and aluminium fin plate on sink side 76 were filled with Thermal Interface Material (TIM). During the experiments, the internal resistance 77 78 of TEG module was matched with the external electric load (R<sub>L</sub>) ensuring maximum power output. 79 At this condition, the effect of influencing parameters such as interface contact pressure and surface roughness and thermal conductivity of TIM was evaluated. Table 1 provides the details of 80 the TEG TIM test set up. 81



82

Fig. 1(a). A scheme of the experimental set up: 1 – Steel holding plate, 2. Electric heater, 3
– aluminium heat spreader plate, 4 – TEG hot side TIM, 5 – Thermoelectric generator
module, 6 – TEG cold side TIM, 7 – aluminium fin heat sink, 8 – Cooling fan, 9 –
Temperature controller, 10 – Electric contactor, 11 – Electric power source, V –

87 Voltmeter, A – Ammeter, S- Electric switch, RL – Variable external load resistor, Ths –

Heat source temperature (°C), T<sub>h1</sub>, T<sub>h2</sub> and T<sub>h3</sub> – heat spreader temperature sensors, T<sub>c1</sub>,
 T<sub>c2</sub> and T<sub>c3</sub> - fin base plate temperature sensors



Fig. 1(b) 3D view of the schematic for TEG experimental set-up



Fig. 2 Experimental set up

Table 1 Details of the	TEG TIM test setup
------------------------	--------------------

Sl No	Description	Value
	Heat source	
1	Electric heater	240×40x10 mm
2	Steel holding plate	240x40x10 mm
3	Aluminum heat spreader plate	240x77x10 mm
	TEG	
4	P and N junction leg	1.5x1.5x1.5 mm
5	Top and bottom copper connecting bar	3.5x1.5x0.5 mm
6	Top and bottom ceramic plate	40x40x0.75 mm
	Heat sink	
7	Fin base plate	240x77x4 mm
8	Fin thickness	2 mm
9	Fin length	240 mm
10	Fin gap	5 mm
11	Number of fins	8 Nos
	Electric load	
12	External electric load resistor	36x10x0.5 mm

#### 98 **2.1 Experimental variables**

### 99 2.1.1 Interfacial contact pressure

The experimental set-up employed for measuring contact pressure on TIM is shown in Fig. 3 with Table 1 presenting the geometric details. The aluminium fin base plate was joined with heat spreading plate using M4 bolts.

103 Considering the challenges in measuring the interfacial contact pressure, a calibration dataset 104 between bolt torque and contact pressure was created using a pressure measuring film (Fuji film 105 prescale, Type: LLW) between the aluminium plate/fin and TEG. The contact pressure measured

106 for different applied torques is shown in Fig. 4.



108Fig. 3 Top view of the experimental set-up arranged for measuring contact pressure109(dimensions in mm)





#### Fig. 4 Measured contact pressure as a function of applied torque

#### Thermal conductivity of different TIM's 112 2.1.2

The silicon grease and silicone oil were used for this study as a base material with nanoparticles 113 (NPs) such as Multiwall Carbon Nanotube (MWCNT) and copper added in varying proportions 114 to improve the thermal conductivity of the TIM. Silicone grease, a mixture of Silicone grease with 115 116 0.5 weight percentage (%wt) of MWCNT and a mixture of Silicone oil with 40 %wt of Cu NPs are respectively shown in Fig. 5(a), 5(b) and 5(c). Their thermal conductivity was measured using 117 Laser Flash Apparatus (LFA 457 microflash<sup>®</sup>, Netzsch, Germany) and are presented in Table 2. 118





Fig. 5 Thermal Interface Materials (TIMs) employed in this study

Sl No	Thermal Interface Material	Thermal conductivity (k <sub>tim</sub> ) (W/m.K)
1	Silicone grease	0.6
2	Silicone grease + 0.5 %wt MWCNT	0.9
3	Silicone Oil + 40 %wt Cu NP	4.2

122 2.1.3 Surface Roughness of base and TEG surface material

123 The aluminium heat spreader plate and aluminium fin base plate used in the experiments had three 124 variations in surface roughness viz.,  $0.8 \mu$ ,  $3.12 \mu$  and  $6 \mu$  as measured by White Light

125 Interferometer (Rtec instruments, USA). The surface roughness of TEG was constant at 1.3  $\mu$ .

#### 126 **3 Modelling**

#### 127 **3.1** Governing equation for Numerical model (NM)

#### 128 **3.1.1.** Heat exchanger model

Energy equation (Laplace equation) for thermoelectric modules for various temperature fields isdescribed in Eq. (1).

$$131 \quad \nabla . \nabla T_{hs} = 0 \tag{1}$$

- 132 where  $T_{hs}$  is the heat source surface temperature
- 133 Temperature of the exposed heat source surface  $(T_{hs})$  was used as the boundary condition. Rate of
- heat transferred from cold side of TEGs ( $Q_c$  in W) by convection was calculated using Eq. (2).

135 
$$Q_c = h_{camb} A_{eff} (T_{hs} - T_a)$$
(2)

136 where  $h_{camb}$  is the heat transfer coefficient between fin and ambient,  $A_{eff}$  is the fin effective area,

137  $T_a$  is the ambient temperature.

#### 138 **3.1.2 Thermal contact model**

Eqs. (3) and (4) provide the conductance (h) at the interface of two bodies in contact [23].

140 
$$-n_d \cdot (-k_d \nabla T_d) = -h(T_u - T_d)$$
 (3)

141 
$$-n_u \cdot (-k_u \nabla T_u) = -h(T_d - T_u)$$
 (4)

where u and d subscripts denote the upside and downside of the slit respectively, k denotes the thermal conductivity, T is the temperature, n is the normal vector to the boundary and the conductance (h) at the interface of two bodies in contact can be written Eq. (5) 145  $h = h_c + h_g$ 

- 146 where  $h_c$  is the contact conductance and  $h_g$  the gap conductance.
- 147 The contact conductance (h<sub>c</sub>) described by Eq. (6) is the heat flux across the surfaces in contact148 [24].

149 
$$h_{c} = \frac{1}{R_{c}A_{a}} = 1.25k_{s} \left(\frac{m_{s}}{\sigma}\right) \left(\frac{P_{tim}}{H_{c}}\right)^{0.95}$$
(6)

where  $R_c$  is the thermal interface resistance due to contact,  $A_a$  is the apparent contact area of joining surfaces,  $P_{tim}$  the contact pressure and  $H_c$  the micro-hardness of softer contact surface of the two surfaces in contact.

153 The effective Root Mean Square (RMS) of surface roughness ( $\sigma$ ) is given as:

154 
$$\sigma = \sqrt{\sigma_{Al}^2 + \sigma_{teg}^2}$$
(7)

155  $\sigma_{Al}$  is the surface roughness plate in contact with TEG,  $\sigma_{teg}$  is the surface roughness of TEG

m<sub>s</sub> is the absolute mean asperity slope obtained from slopes  $m_{Al}$  and  $m_{teg}$  for two contacting surfaces. The effective absolute mean asperity slope (m<sub>i</sub>) is obtained using Eq. (8).

158 
$$m_i = 0.152(\sigma_i)^{0.44}$$
 (8)

159 where  $\sigma_i$  is the effective absolute surface roughness

$$160 \qquad m_s = \sqrt{m_{Al}^2 + m_{teg}^2}$$

161 Then, the thermal conductivity of the material,  $k_s$  [23], could be calculated using Eq. (9).

162 
$$\frac{2}{k_s} = \frac{1}{(k_u n_u) \cdot n_u} + \frac{1}{(k_d n_d) \cdot n_d}$$
 (9)

where u and d subscripts denote the upside and downside of the slit refer respectively, k denotesthe thermal conductivity and n is the normal vector to the boundary.

165 For parallel plate, gap conductance (hg) could be calculated by using Eqs. (10) - (13) [23 and 24].

166 
$$h_g = \frac{1}{R_g A_a} = \frac{k_{tim}}{Y + M}$$
 (10)

where Y is the layer thickness of the TIM,  $R_g$  is the thermal interface resistance due to gap and k<sub>tim</sub> is the thermal conductivity of TIM.

169 According to simple power law relation [17], the mean plane separation Y will be

170 
$$Y = 1.53\sigma \left(\frac{P_{tim}}{H_c}\right)^{-0.097}$$
 (11)

171 M = 0, for TIM filled gap,

172 where M is a constant and  $M = \alpha_a \beta \wedge$ , for the gap filled by air ( $k_{tim} = k_{air}$ ). (13)

(12)

173 For air, gas parameters  $\alpha_a = 2.4$ ,  $\beta = 1.7$  and molecular free path ( $\wedge$ ) = 0.06  $\mu$ m.

174 The thermal interface conductance h for both hot and cold sides of TEG could be found by using

175 Eqs. (5) - (13).

#### 176 **3.1.3 Coupled field model**

Accounting for the coupling mechanisms of Seebeck, Peltier and Thomson effects between
electrical and thermal fields, a fully coupled-field model was developed by generating governing
equations under steady-state conditions for both electrical potential profiles and temperature in
the absence of input magnetic field [25].

By taking Joule heating into account in the process, the equation for energy conservation is givenby

183 
$$\nabla (\mathbf{k} \cdot \nabla \mathbf{T}) - \mathbf{T} \cdot \mathbf{J} \cdot \frac{\partial \alpha}{\partial \mathbf{T}} + \rho \cdot \mathbf{J} = 0$$
(14)

184 where  $\rho$  is the electrical resistivity, k is the thermal conductivity of TEG leg, T is the temperature, 185 J is the current density and  $\alpha$  is the Seebeck coefficient.

186 Now, applying thermoelectric effect into the coupling of heat flow equation and electric charge187 continuity equation [25],

$$188 \quad \nabla . J = 0 \tag{15}$$

189 
$$q = [\Pi] \cdot J - [k] \cdot \nabla T$$
 (16)

190 
$$\mathbf{J} = [\sigma_e] \cdot (\mathbf{E} - [\alpha] \cdot \nabla \mathbf{T})$$
(17)

where  $[\sigma_e]$  is the electrical conductivity of TEG leg matrix, [k] is the thermal conductivity of TEG leg matrix,  $[\alpha]$  is the Seebeck coefficient of TEG leg matrix and  $[\Pi]$  is the Peltier coefficient of TEG leg matrix which depends on T $[\alpha]$ 

- 194 In the absence of time varying magnetic field, E becomes irrotational and was derived from an
- 195 electric scalar potential ( $\phi$ )

$$196 \quad E = -\nabla \phi \tag{18}$$

197 Hence, electric power (P<sub>o</sub>) expression is given by

198 
$$P_o = \frac{V_{oc}^2}{2(R_{teg} + R_L)}$$
 (19)

- where  $V_{oc}$  is the open circuit voltage,  $R_{teg}$  is the internal resistance of TEG,  $R_L$  is the external load resistance.
- 201 For obtaining maximum electric power,  $R_L = R_{teg}$
- 202 The thermoelectric equations provided above were used for determining the five state vector
- 203 parameters  $Q_h$ ,  $Q_c$ ,  $T_h$ ,  $T_c$  and  $I_o$  for TEGs.

#### **3.2** Computer model and the boundary conditions employed

A 3D TEG system (see Table 1 for geometric details), was modelled using COMSOL<sup>TM</sup>

206 Multiphysics for cold and hot side thermal contact resistance. Fig. 6 shows the 3D mesh for the

207 overall TEG system employed. A 3D mesh (Fig. 6(a)) and a fine mesh (Fig. 6(b)) were used in

the TEG P and N junction elements to capture a realistic thermoelectric effect.





Fig. 6(a) 3D mesh for TEG system of TIM

Fig. 6(b) Zoomed mesh TEG P and N junction elements

- Principles of heat transfer in solids, thermoelectric effect and Yovanovich correlation [24] were
  employed in the analysis. Table 3 provides the material properties and Table 4 the boundary
  conditions employed.
- 212
- 213
- 213
- 214

Table 3 Material properties of the TEG-TIM components employed

SI No	Description	Value
	Base plate and heat sink	
1	Thermal conductivity of aluminum base plate	201 W/mK
2	Thermal conductivity of aluminum heat sink	201 W/mK
	TEG	

3	Thermal conductivity of top and bottom alumina plate	40 W/mK
4	Thermal conductivity of top and bottom copper bar	401 W/mK
5	Seebeck coefficient of P-junction	0.0002 V/K
6	Seebeck coefficient of N-junction	0.0002 V/K
7	Thermal conductivity of P-junction	1.7 W/mK
8	Thermal conductivity of N-junction	1.7 W/mK
9	Resistivity of P-junction	1X10 <sup>-5</sup> Ωm
10	Resistivity of N-junction	1X10 <sup>-5</sup> Ωm
11	Resistivity of top and bottom copper bar	2.27X10 <sup>-8</sup> Ωm



#### Table 4 Boundary conditions employed

Sl No	Description	Value
1	Base plate hot source temperature (T <sub>hs</sub> )	100, 150, 200 °C
2	Surface roughness of TEG ( $\sigma_{teg}$ )	1.3 μ
3	Surface roughness of aluminium base and fin $(\sigma_{Al})$	0.8, 3.1,6 µ
4	Contact pressure (P <sub>tim</sub> )	420, 840, 1240,1650 kPa
5	Surface hardness of aluminium material $(H_{Al})$	1060 MPa
6	Ambient temperature (T <sub>a</sub> )	35°C
7	Combined heat transfer co-efficient (fin surface to	25 W/m <sup>2</sup> K
	ambient) (h <sub>camb</sub> )	
8	Low potential on N-junction bottom copper bar	0 V
9	Electric conductivity of electric load resistor at 200	2955, 2585, 2501 S/m
	°C, 150 °C, 100 °C for TEG internal resistance equal	
	to load resistance	

#### 216 **3.3 Performance coefficients of TEG**

217 Seebeck effect states that for an electrical conductor, the temperature difference across the 218 conductor will cause the induction of an electric current and TEG works using this principle. In 219 addition, Peltier effect, Fourier effect and Joule effect also play a significant role in a TEG module.

TEG performance can be described by considering the Seebeck coefficient, its internal electrical resistance and thermal conductance. The hot side thermal power input ( $Q_h$  in W) and the cold side thermal power output ( $Q_c$  in W) were calculated by using Eqs. (20) - (29) [26].

223 
$$Q_h = \alpha I_o T_h + K(T_h - T_c) - \frac{I_o^2 R_{teg}}{2}$$
 (20)

224 
$$Q_c = \alpha I_o T_c + K(T_h - T_c) + \frac{I_o^2 R_{teg}}{2}$$
 (21)

- where T<sub>h</sub> is the TEG hot side temperature, T<sub>c</sub> is the TEG cold side temperature, I<sub>o</sub> is the output 225 current and 226 227  $\alpha$  is the Seebeck coefficient (V/K) of the TEG module can be described as:  $\alpha = N_c \alpha(T)$ (22)228 where N<sub>c</sub> is module series connected couple count and  $\alpha(T)$  is the Seebeck coefficient of the P-N 229 couple 230 The internal resistance  $(R_{teg})$  of the TEG module is given by 231  $R_{\text{teg}} = \frac{N_c L \rho(T)}{A_{ct}}$ 232 (23) where L is the height of P-type and N-type elements and Act the cross-sectional area of P-type / 233 N-type elements and  $\rho(T)$  is the electrical resistivity of the P-N couple 234 The thermal conductance (K) of the TEG module is given as 235  $K = \frac{N_c A_{ct} k(T)}{H_1}$ 236 (24)237 where k(T) is the thermal conductivity of the P-N couple and H<sub>1</sub> is the height of the TEG element The power generated by the TEG system was calculated from heat flux variation or from the 238 product of voltage and output current. 239  $P_{o} = V_{o}I_{o} = Q_{h} - Q_{c}$ (25)240 where  $P_0$  is the electric power output and  $V_0$  is the output voltage 241 Using Eq. (20) and Eq. (21), Eq. (25) can be written as 242  $P_{o} = Q_{h} - Q_{c} = \alpha I_{o}(T_{h} - T_{c}) - I_{o}^{2}R_{teg}$ (26)243 The output voltage can be found from Eq. (26) 244  $V_{o} = \frac{P_{o}}{I_{o}} = \alpha(T_{h} - T_{c}) - I_{o}R_{teg}$ (27)245 During open circuit condition (I<sub>0</sub>=0), open circuit voltage (V<sub>oc</sub>) can be deduced from Eq. (27) as 246 shown in Eq. (28). 247  $V_{oc} = \alpha (T_h - T_c)$ (28)248
  - Hence, the output current (I<sub>o</sub>) was calculated by 1<sup>st</sup> order partial derivative of Eq. (26) and equating 249 it to zero. 250

251 
$$I_o = \frac{V_{oc}}{R_g + R_L} = \frac{\alpha(T_h - T_c)}{R_g + R_L}$$
 (29)

where  $R_L$  is the variable electrical load resistance connected externally to the circuit.

#### 253 **3.4 Heat Transfer model of TEG with TIM's.**

In this study, the A plate fin heat sink with a fan on the cold side was used to minimize the TEG cold side temperature.

The developed heat transfer model accounted for the thermal interface resistances of hot and cold sides of TEG. Thermal resistance on hot side comprised of interface thermal resistance ( $R_{hi}$ ) and heat spreading plate thermal resistance ( $R_{sp}$ ). Thermal resistance on cold sides comprised of interface thermal resistance ( $R_{ci}$ ), fin base plate thermal resistance ( $R_{bf}$ ) and fin to air convective thermal resistance ( $R_{camb}$ ).

The thermal resistances of the system from hot side to cold side of the TEG are as shown in Fig.7.





264

#### Fig. 7 Details on thermal resistances of TEG system



266 
$$R_{sp} = \frac{t_{sp}}{k_{sp}A_{sp}} = \frac{t_{sp}}{k_{sp}W_{sp}L_{sp}}$$
(30)

where  $R_{sp}$  is the thermal resistance of heat spreader plate,  $k_{sp}$ ,  $t_{sp}$ ,  $A_{sp}$ ,  $W_{sp}$  and  $L_{sp}$  are the thermal conductivity, thickness, surface area, width and length of the heat spreader plate respectively.

- 269 Introduction of the TIM reduces air gap and increases thermal conductivity and hence reduces the
- 270 temperature difference contact surfaces. The following factors influence the interface resistances
- 271 on hot and cold sides of  $TEG_{\overline{}}$ :
- 272 1. Thermal conductivity of TIM  $(k_{tim})$
- 273 2. Surface roughness ( $\sigma$ )
- 274 3. Contact pressure  $(P_{tim})$

The contact and gap resistances ( $R_c$  and  $R_g$ ) of hot and cold side of TEG could be obtained using Eqs. (5) - (13). The combined resistances of hot ( $R_{hi}$ ) or cold ( $R_{ci}$ ) side could be obtained using

277 Eq. (31).

278 
$$\frac{1}{R_i} = \frac{1}{R_c} + \frac{1}{R_g}$$
 (31)

- The total interface resistance  $(R_i)$  is expressed as in Eq. (31) considering the following assumptions:
- 1. The surfaces are microscopically rough and macroscopically conforming.
- 282 2. The plastic deformation occurs in the softer solid and the flow pressure is constant.
- 283 3. The contact spots are isothermal.
- 4. The total heat flow rate through each flux tube can be separated into two independent heat flowrates: contact spot and gap flow rates.
- 5. The effective gap thickness is dependent upon the surface roughness and the relative contactpressure.
- 288 6. Non-continuum gas effects must be taken into account.
- 289 7. The surfaces are clean and free from oxides, films, etc.
- 290 8. Radiative heat transfer is negligible.
- 291 The fin base plate resistance  $(R_{fb})$  could be expressed as

292 
$$R_{fb} = \frac{t_{fb}}{k_{fb}A_{fb}} = \frac{t_{fb}}{k_{fb}W_{fb}L_{fb}}$$
 (32)

where  $R_{fb}$  is the fin base plate thermal resistance,  $k_{fb}$ ,  $t_{fb}$ ,  $A_{fb}$ ,  $W_{fb}$  and  $L_{fb}$  are the thermal conductivity, thickness, surface area, width and length of the fin base plate respectively.

Ambient thermal resistance  $(R_{camb})$  could be expressed as

296 
$$R_{camb} = \frac{1}{h_{camb}A_{eff}}$$
(33)

297 where  $h_{camb}$  is the combined heat transfer co-efficient which could be expressed as,

298 
$$h_{camb} = 5.678 \left\{ a + b \left[ \frac{(294.26V_w/(T_a))}{0.3048} \right]^n \right\}$$
 (34)

- 299 where a = 0.99, b = 0.21, n=1 for  $V_w < 4.88$  m/s
- 300 a = 0, b = 0.5, n=0.7 for  $4.88 \le V_w \ge 30.48$  m/s
- and  $V_w$  is the wind velocity,  $T_a$  is the ambient temperature
- For plate fin heat sink effective heat transfer area ( $A_{eff}$ ) and fin efficiency ( $\eta_f$ ) could be obtained
- 303 by using Eqs. (35) (37).
- 304 Plate fin heat sink effective heat transfer area,

305 
$$A_{eff} = (\eta_f (2N_f L_f H_f) + (N_f - 1)bL_f)$$
 (35)

where  $N_f$  is the number of fin,  $L_f$  is the length of the fin,  $H_f$  is the height of the fin, b is the tunnel width.

308 Fin efficiency, 
$$\eta_f = \frac{\tanh(mH_f)}{mH_f}$$
 (36)

$$309 \qquad m = \sqrt{\frac{h_{camb}Xp}{k_f Xt_f}} \tag{37}$$

- where p is the perimeter of the fin tip,  $k_f$  is the thermal conductivity of fin and  $t_f$  is the thickness of the fin.
- U<sub>h</sub>, A<sub>h</sub> and U<sub>c</sub>, A<sub>c</sub> are overall heat transfer coefficient and effective heat transfer area on hot and
  cold side respectively could be obtained by using Eqs. (38) and (39).

$$314 \qquad U_h A_h = \frac{1}{R_{sp} + R_{hi}} \tag{38}$$

315 
$$U_c A_c = \frac{1}{R_{ci} + R_{fb} + R_{camb}}$$
 (39)

The heat supplied (Q<sub>h</sub>) to hot side and heat dissipated (Q<sub>c</sub>) out through cold side were given by the equations:

318 
$$Q_h = U_h A_h (T_{hs} - T_h)$$
 (40)

319 
$$Q_c = U_c A_c (T_c - T_a)$$
 (41)

By equating Eq. (20) with Eq. (40) and Eq. (21) with Eq. (42), the expressions for  $T_h$  and  $T_c$  were arrived as follows:

322 
$$T_{\rm h} = \frac{U_{\rm h}A_{\rm h}T_{\rm hs} + KT_{\rm c} + \frac{I_0^2R_{\rm teg}}{2}}{\alpha I_{\rm o} + K + U_{\rm h}A_{\rm h}}$$
 (42)

323 
$$T_{c} = \frac{U_{c}A_{c}T_{a} + KT_{h} + \frac{I_{0}^{2}R_{teg}}{2}}{U_{c}A_{c} + K - \alpha I_{0}}$$
(43)

where  $U_c$  is the overall heat transfer coefficient on cold side and  $U_{h is}$  the overall heat transfer coefficient on hot side.

Th and T<sub>c</sub> were iteratively computed for different source temperatures and other variables. The expression for I<sub>o</sub> was obtained by substituting T<sub>hs</sub>, T<sub>a</sub>,  $\alpha$  and R<sub>teg</sub> into Eq. (29). Consequently, Q<sub>h</sub>, Q<sub>c</sub>, P<sub>o</sub> and V<sub>o</sub> expressions were obtained by substituting T<sub>h</sub>, T<sub>c</sub>,  $\alpha$ , R<sub>teg</sub>, K and I<sub>o</sub> into Eqs. (20), (21), (42) and (43).

#### 330 4 Results and discussion

#### 331 4.1 Modelling analysis

The commercially available COMSOL<sup>TM</sup> multiphysics numerical model having in-built governing equations discussed in 3.1 was simulated for all material properties and boundary conditions of TEG-TIM test set up as given in Table 3 and Table 4 respectively. Outputs at both open and closed circuit conditions were obtained for each variation.

Fig. 8(a) and 9(a) show the temperature and open circuit voltage contours respectively for a case with no TIM (only air gap) and  $T_{hs} = 200 \text{ °C}$ ,  $\sigma = 1.53 \mu$  and  $P_{tim} = 1650 \text{ kPa}$ .

Fig. 8(b) and 9(b) show the temperature and open circuit voltage contours respectively for a case with Silica oil + 40 %wt Cu nanoparticle as TIM and  $T_{hs} = 200$  °C,  $\sigma = 1.53 \mu$  and  $P_{tim} = 1650$ kPa.

Maroon colour shows the highest temperature/voltage while blue colour indicates lowest temperature/voltage in the above pictures. Comparison of the colour contours with and without TIM in the interface zone between the top of TEG and the bottom of fin plate and that between the bottom surface of TEG and top of hot plate reveal appreciable reduction in temperatures at the interfaces due to the introduction of TIM leading to an increased open circuit voltage in the output. Similar improvement is seen in the contours for closed circuit.



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Fig. 8(a) Temperature contour at open circuit condition for no TIM (only entrapped air) and  $T_{hs} = 200 \text{ °C}$ ,  $\sigma = 1.53 \mu$  and  $P_{tim} = 1650 \text{ kPa}$ 



Fig. 8(b) Temperature contour at open circuit condition for Silica Oil+ 40% Cu

352 Nanoparticle ( $k_{tim} = 4.2 \text{ W/mK}$ ) as TIM and $T_{hs} = 200 \text{ °C}$ , $\sigma =$
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Fig. 9(a) Voltage contour at open circuit condition for no TIM (only entrapped air) and T<sub>hs</sub> = 200 °C,  $\sigma$  = 1.53  $\mu$  and P<sub>tim</sub> = 1650 kPa



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## Fig. 9(b) Voltage contour at open circuit condition for Silica Oil+ 40% Cu Nanoparticle (k<sub>tim</sub> = 4.2 W/mK) as TIM and T<sub>hs</sub> = 200 °C, $\sigma$ = 1.53 $\mu$ and P<sub>tim</sub> = 1650 kPa

Fig. 10(a) and 11(a) show the temperature and closed circuit voltage contours respectively for a case with no TIM (only air gap) and  $T_{hs} = 200 \text{ °C}$ ,  $\sigma = 1.53 \mu$  and  $P_{tim} = 1650 \text{ kPa}$ .

Fig. 10(b) and 11(b) show the temperature and closed circuit voltage contours respectively for a

363 case with Silica oil + 40 %wt Cu nanoparticle as TIM and  $T_{hs} = 200$  °C,  $\sigma = 1.53 \mu$  and  $P_{tim} =$ 

364 1650 kPa.









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Fig. 10(b) Temperature contour at closed circuit condition for Silica Oil+ 40% Cu
Nanoparticle (k<sub>tim</sub> = 4.2 W/mK) as TIM and T<sub>hs</sub> = 200 °C, σ = 1.53 μ and P<sub>tim</sub> = 1650 kPa



Fig. 11(a) Voltage contour of closed circuit condition for no TIM (only entrapped air) and  $T_{hs} = 200 \text{ °C}, \sigma = 1.53 \mu \text{ and } P_{tim} = 1650 \text{ kPa}$ 



- 376
- 377 Fig. 11(b) Voltage contour of closed circuit condition for Silica Oil+ 40% Cu Nanoparticle

( $k_{tim} = 4.2 \text{ W/mK}$ ) as TIM and  $T_{hs} = 200 \text{ °C}$ ,  $\sigma = 1.53 \mu$  and  $P_{tim} = 1650 \text{ kPa}$ 

# 4.2 Comparison of the model outputs with experimental data and evaluation of the impact of various parameters on the performance of TEG

Experiments and model outputs for varying thermal conductivities of 0.025, 0.6, 0.9 and 4.2
W/mK for TIM at hot side temperatures of 100, 150 and 200 °C, contact pressures of 420, 840,
1240 and 1650 kPa and surface roughness of 0.8, 3.1 and 6µ were compared for open circuit
voltage and power output of TEG.

385

#### 4.2.1 Influence of thermal conductivity

Fig. 12 and Fig. 13 show typical trends of open circuit voltage and closed circuit power outputs 386 of TEG with respect to thermal conductivity of TIM keeping the other variables constant as shown 387 in the respective figures. Analysis of the trends indicates steep increase in voltage and power 388 outputs upto a thermal conductivity of 0.6 W/mK compared with that of air having a thermal 389 conductivity of 0.025 W/mK and subsequent increase in outputs are very little for the increases in 390 thermal conductivities to 0.9 and 4.2 W/mK. Though the trends of outputs of both models are in 391 line with experimental data, the outputs of COMSOL<sup>TM</sup> model is in close agreement with 392 experiments with marginal deviation in the range 0.3 to 2.6 % for open circuit voltage and 0.5 to 393 3.1 % for electric power output. The outputs of heat transfer model comparatively deviate in the 394 range of 2.3 to 5.9 % for open circuit voltage and 3.3 to 11.3 % for electric power output when 395 compared to the experimental data. 396

397 It is clear from the data that the TIM fills up the unnoticeable surface undulations, establishes 398 better connectivity and conductivity between the mating surfaces and thus improves the performance of TEG by 10 to 20%. The data has also revealed that the use of TIM with a thermal
conductivity higher than 0.6 W/mK has only marginal improvement in the performance.

#### 401 **4.2.2 Influence of contact pressure**

Fig. 14 and Fig. 15 show typical trends of open circuit voltage and closed circuit power outputs of TEG with respect to contact pressure between the spreading plates and TIM keeping the other variables constant as shown in the respective figures. The analysis of the trends indicates progressive improvements in voltage and power outputs at all conditions for a case with no TIM (only entrapped air) and the pressure requirement is higher for a rough surface than a smooth surface. Contact pressure does not have any effect at any condition for TIMs having higher thermal conductivities in the range of 0.6 to 4.2 W/mK.

#### 409 4.2.3 Influence of surface roughness

Fig. 16 and Fig. 17 show typical trends of open circuit voltage and closed circuit power outputs of TEG with respect to surface roughness of heat spreading aluminium plates keeping the other variables constant as shown in the respective figures. The analysis indicated that the surface roughness is influential only when air is used as TIM and not for other TIMs having higher thermal conductivities.

#### 415 **4.2.4 Influence of heat source temperature**

Fig. 18 and Fig. 19 show typical trends of open circuit voltage and closed circuit power outputs of TEG with respect to hot side temperatures keeping the other variables constant as shown in the respective figures. The results indicate that irrespective of the TIM, the open circuit voltage and electric power output keep increasing with increase in source temperature. However, the outputs are higher with the use of TIMs with higher thermal conductivity than air.

421 Recently, Wang et al. [22] analysed the performance of TEG with air and thermal grease as TIM under varying contact pressures of up to 765 kPa, however, the effect of roughness of the contact 422 423 surfaces was ignored. This aspect has been covered by the present study and approximately 12% increase in power output with the use of TIM (2.01 W with air to 2.25 W with TIM at a contact 424 425 pressure of 420 kPa) is being reported. Wang et al. [22] reported an increase in power output with an increase in contact pressure even when TIM was used. Whereas, what this paper reports here 426 is an increase in power output with an increase in contact pressure only with air and it remains 427 almost constant at all contact pressures when TIM is used. 428





Fig. 12 Influence of thermal conductivity of TIM at open circuit condition



Fig. 13 Influence of thermal conductivity of TIM at closed circuit condition





Fig. 14 Influence of contact pressure and TIM at open circuit condition





Fig. 15 Influence of contact pressure and TIM at closed circuit condition

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Fig. 16 Influence of surface roughness and TIM at open circuit condition





Fig. 17 Influence of surface roughness and TIM at closed circuit condition







Fig. 19 Influence of heat source temperature at closed circuit condition

#### 450 5 Conclusions

Experiments were carried out with different Thermal Interface Materials (TIM) of different thermal conductivities at varying conditions of contact pressure, surface roughness and heat source temperature. Mathematical Heat Transfer Model and numerical model using COMSOL<sup>TM</sup> Multiphysics were developed and validated with the experimental results. The impacts of thermal conductivity, contact pressure, surface roughness and heat source temperature on the thermal performance of TIM and in turn the performance of TEG were evaluated.

457 The following are the observations:

- A TIM material having a thermal conductivity of 0.6 W/mK was found to be the best;
  increasing the thermal conductivities to 0.9 and 4.2 W/mK did not have appreciable
  increase in voltage and power output from TEG. Hence, use of expensive TIMs comprising
  MWCNT and Cu NPs may not be required.
- 462 2. Increase in contact pressure improves voltage and power outputs at all conditions for a
  463 case when no TIM (only entrapped air) is used. It does not have any effect at any condition
  464 for TIMs having higher thermal conductivities of 0.6, 0.9 and 4.2 W/mK.
- 3. Increase in surface roughness decreases the voltage and power output at all conditions for
  a case when no TIM (only entrapped air) is used. Surface roughness effect is insignificant
  for TIMs having higher thermal conductivities of 0.6, 0.9 and 4.2 W/mK.
- 468
  4. Increase in source temperature increases the voltage and power output irrespective of the
  469
  469 TIM used. For the same source temperature, the outputs increase with increase in thermal
  470
  470
- 5. The trends of the outputs of both COMSOL<sup>TM</sup> and Heat Transfer Models (HTM) were in
  line with the observations of experiments. However, the outputs of COMSOL<sup>TM</sup>
  Multiphysics model had a closer agreement with experimental observation than that of
  mathematical heat transfer model.

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#### 549 Nomenclature

Aa	apparent contact area of joining surfaces (m <sup>2</sup> )
Ac	effective heat transfer area on cold side $(m^2)$
Act	total cross-sectional area of P-type / N-type elements (m <sup>2</sup> )
$A_{\text{eff}}$	fin effective area $(m^2)$
$A_{fb}$	surface area of the fin base plate (m <sup>2</sup> )
$A_h$	effective heat transfer area on hot side (m <sup>2</sup> )
$A_{sp}$	surface area of the heat spreader plate (m <sup>2</sup> )
b	tunnel width (m)
E	magnetic field (V)
h	combined thermal interface conductance (W/m <sup>2</sup> K)
hc	contact conductance $(W/m^2K)$
H <sub>c</sub>	micro-hardness of softer contact surface of the two surfaces in contact (MPa)
$h_{\text{camb}}$	heat transfer coefficient between fin and ambient (W/m <sup>2</sup> K)
$H_{f}$	height of the fin (m)
hg	gap conductance (W/m <sup>2</sup> K)
$H_1$	height of the TEG element (m)
Io	output current (A)
J	TEG current density (A/m <sup>2</sup> )
k	thermal conductivity (W/mK)

Κ	thermal conductance (W/K)
$\mathbf{k}_{\mathbf{f}}$	thermal conductivity of fin (W/mK)
$k_{fb}$	thermal conductivity fin base plate (W/mK)
ks	harmonic mean mean of two contacting surfaces thermal conductivity (W/mK)
$\mathbf{k}_{sp}$	thermal conductivity of the heat spreader plate (W/mK)
$\mathbf{k}_{tim}$	Thermal conductivity of TIM (W/mK)
k(T)	thermal conductivity of the P-N couple (W/mK)
L	height of P-type and N-type elements (m)
$L_{\mathrm{f}}$	length of the fin (m)
L <sub>fb</sub>	length of the fin base plate (m)
$L_{sp}$	length of the heat spreader plate (m)
ms	absolute mean asperity slope
mi	effective absolute mean asperity slope
n	normal vector to the boundary
Nc	number of couple in TEG (No)
$N_{\mathrm{f}}$	number of fin (No)
p	perimeter of the fin tip (m)
Po	electric power output (W)
P <sub>tim</sub>	contact pressure (MPa)
Qc	Rate of heat transferred from cold side of TEG (W)
$Q_h$	heat absorption by TEG (W)
R <sub>c</sub>	thermal interface resistance due to contact (m <sup>2</sup> K/W)
R <sub>ci</sub>	combined resistances of TEG cold side interface (m <sup>2</sup> K/W)
$R_{camb}$	ambient thermal resistance (m <sup>2</sup> K/W)
$R_{\mathrm{fb}}$	fin base plate thermal resistance $(m^2K/W)$
$R_{g}$	thermal interface resistance due to gap (m <sup>2</sup> K/W)
$R_{hi}$	combined resistances of TEG hot side interface (m <sup>2</sup> K/W)
$R_L$	external load resistance ( $\Omega$ )
$R_{sp}$	thermal resistance of heat spreader plate (m <sup>2</sup> K/W)
R <sub>teg</sub>	TEG internal resistance ( $\Omega$ )
Ta	ambient temperature (K)
t <sub>f</sub>	thickness of the fin (m)
t <sub>fb</sub>	thickness of the fin base plate (m)
$T_{hs}$	heat source surface temperature (K)

Т	temperature (K)
$T_h$	TEG hot side temperature (K)
Tc	TEG cold temperature (K)
t <sub>sp</sub>	thickness of the heat spreader plate (m)
Uc	overall heat transfer coefficient on hot side (W $/m^2K$ )
$U_h$	overall heat transfer coefficient on hot side (W $/m^2K$ )
Vo	TEG output voltage (V)
V <sub>oc</sub>	TEG open circuit voltage (V)
$V_{\rm w}$	wind velocity (m/s)
$W_{fb}$	width of the fin base plate (m)
$W_{sp}$	width of the heat spreader plate (m)
Y	layer thickness of the TIM (m)
[k]	thermal conductivity of TEG leg matrix (W/mK)
Greek syn	nbol
α	Seebeck coefficient of TEG module (V/K)
[α]	Seebeck coefficient of TEG leg matrix (V/K)
$\alpha_a$ and $\beta$	gas parameters
<b>α</b> (T)	Seebeck coefficient of the P-N couple (V/K)
$\wedge$	molecular free path (m)
φ	electric scalar potential (V)
$\eta_{\rm f}$	fin efficiency (%)
ρ	electrical resistivity (Ωm)
<b>ρ</b> (T)	electrical resistivity of the P-N couple ( $\Omega m$ )
[Π]	Peltier coefficient of TEG leg matrix which depends on $T[\alpha]  (W/A)$
σ	effective RMS surface roughness (m)
$\sigma_{Al}$	Surface roughness of base plate material surface (m)
σe	electrical conductivity of TEG leg matrix (S/m)
$[\sigma_e]$	electrical conductivity of TEG leg matrix (S/m)
$\sigma_{i}$	effective absolute surface roughness (µ)
$\sigma_{teg}$	Surface roughness of TEG module surface (m)
Subscript	
d	downside of the slit

u

upside of the slit