Composite Thermoelectric Devices

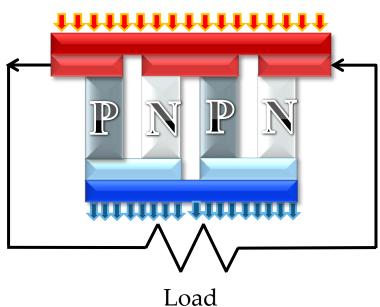
Minking Chyu, Leighton and Mary Orr Chair Professor and Chairman B. V. K. Reddy, Post-Doc Researcher Matthew Barry, Graduate Research Assistant John Li, Adjunct Faculty

Department of Mechanical Engineering and Materials Science University of Pittsburgh

Conventional TEDs

Power Generation

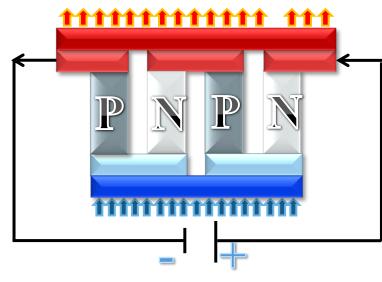
Waste Heat Source



Heat Rejected to Environment

Heat Rejected to Environment

Refrigeration



Power Source

Heat Removed From Refrigerated Space

Heat Transfer Direction in TE Device:

Intended

Natural

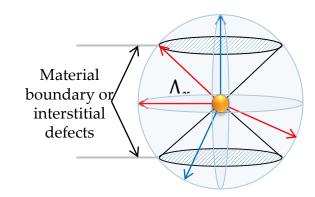






Approaches and Opportunities

- Improve intrinsic <u>material</u> properties for higher ZT via doping and interstitial defects
 - Increasing the power factor through:
 - Complex crystal structures (Phonon-glass electron crystal approach)
 - Dopant-Enhancement of density of states (DOS) near the Fermi level
 - Decreasing the thermal conductivity through:
 - Heavy element compounds
 - Alloy point defect scattering
 - Increasing the presence of interfaces and surfaces to enhance phonon scattering
 - Leading to higher ZT

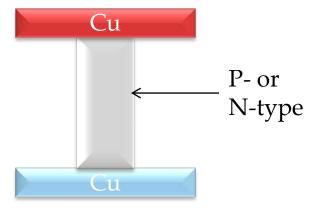


- Improve <u>system</u> performance η or COP, equivalent to higher *effective* ZT
 - By creating stackable thin-film thermoelectric devices, utilizing superlattice and/or quantum effects to reduce thermal conductivity while increasing ZT
 - By employing geometric restructuring, such as heterogeneous composite design, substantially higher equivalent ZT and performance can be achieved
 - By implementing effective system integration for enhanced overall performance

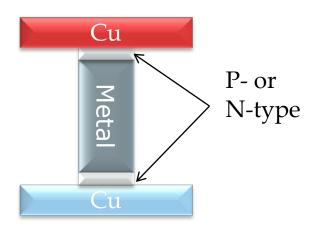
Composite Thermoelectric Devices

- Composite thermoelectric element:
 Semiconductor plates laminated with a highly electrically and thermally conducting material
- Composite approach effectively optimize the collective thermoelectric properties to reduce the Ohmic heating and increase the power output and equivalent ZT values
- Reduction in rare-earth metals usage

Power output
$$P_0 = I^2 R_0$$
 $I = \frac{\alpha \Delta T}{R + R_0}$
Heat recovery efficiency $\eta = \frac{P_0}{Q_H} = \frac{P_0}{K\Delta T + \alpha I T H - \frac{1}{2} I^2 R}$



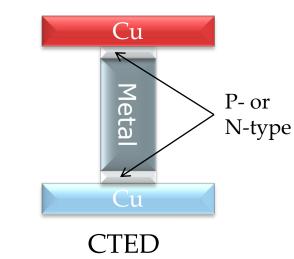
Conventional

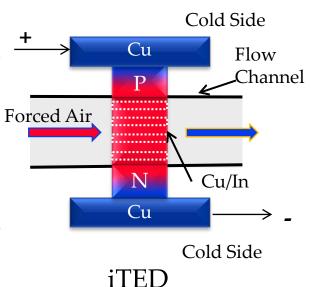


Composite

Integrated Thermoelectric Devices (iTEDs)

- Major part of the semiconductor material is replaced with a conductor along with flow channels drilled through it.
- This configuration also acts as a low thermal resistance heat exchanger eliminating the thermal resistances attributed to the heat sinks.
- Helps to enhance heat transfer on the hot side.
- Eliminate thermal resistance between conventional Cu/ceramic heat-exchanger interface
- Reduce heat flow-back between elements
- Alleviate potential of stresses/mismatch induced from thermal expansion.

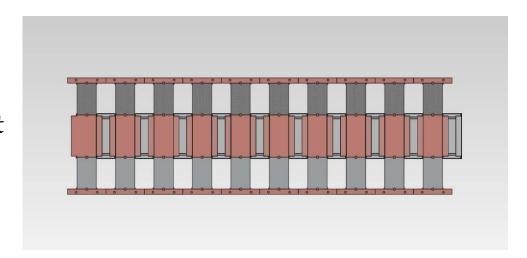




iTEDs

Applications include:

- Waste heat recovery
- Solid-state refrigeration
- ZT doesn't matter if can't take large quantities of heat!

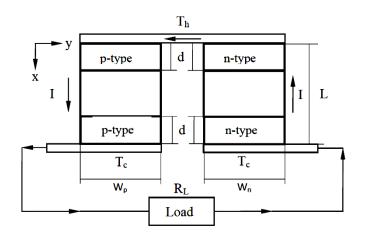


Benefits:

- Scalable
- Can use any TE material
- Can cascade TE materials, or place different material in different flow position to optimize temperature-dependent ZT values
- Can place thin-film materials on top and bottom (C-TED+iTED)

CTED-Analytical Solutions

- Assumptions for Solving temperature profile T(x)
 - Homogeneous and isotropic material properties
 - One-dimensional, steady stat
 - Fourier conduction
 - Ohmic heating
 - Thomson heating
 - Convective heat transfer



Energy equation:

$$\frac{d^2T}{dx^2} + \frac{\rho I^2}{kA^2} - \frac{\tau I}{kA}\frac{dT}{dx} - \frac{hP}{kA}(T - T_{\infty}) = 0$$

$$\theta = \frac{T - T_{cw}}{T_h - T_{cw}}$$

Interface temperatures:

$$\theta_1 = \left[1 + \frac{k_{s2}}{k_c} \frac{(1 - 2\delta)}{(e^{D_2\delta} - 1)} D_2\right] \theta_2 - \frac{k_{s2}}{k_c} \frac{(1 - 2\delta)}{(e^{D_2\delta} - 1)} M_2 \left[e^{D_2\delta} - 1 - \delta D_2\right]$$

$$\theta_2 = \frac{A + M_2 \left[\frac{e^{D_2 \delta} - 1 - \delta D_2}{e^{D_2 \delta} - 1} \right] \frac{k_{s2}}{k_{s1}} \left[e^{-D_1 \delta} - 1 - D_1 \frac{k_{s1}}{k_c} (1 - 2\delta) \right]}{\frac{D_2}{(e^{D_2 \delta} - 1)} \frac{k_{s2}}{k_{s1}} \left[e^{-D_1 \delta} - 1 - D_1 \frac{k_{s1}}{k_c} (1 - 2\delta) \right] - D_1}$$

$$\chi = \frac{I^2 \rho L^2}{kA^2 (T_h - T_{cw})}$$

$$\Gamma = \frac{\tau IL}{kA} \quad \delta = \frac{d}{L}$$

$$D_1 = \Gamma_{s1}, \quad D_2 = \Gamma_{s2}$$

$$M_1 = \left(\frac{\chi}{\Gamma}\right)_{s1} M_2 = \left(\frac{\chi}{\Gamma}\right)_{s2}$$

where
$$A = \chi_c (1 - 2\delta)^2 \left[\frac{k_c}{k_{s1}} \frac{(e^{-D_1\delta} - 1)}{1 - 2\delta} - \frac{D_1}{2} \right] - D_1 [1 + M_1\delta] - M_1 (e^{-D_1\delta} - 1)$$

CTED-Analytical Solutions

Heat transfer at the hot surface:

$$Q_h = \alpha I T_h + \frac{k A (T_h - T_{cw})}{L} \left[\frac{(-1 + \theta_1 - M_1 \delta) D_1}{1 - e^{D_1}} - M_1 \right]$$

Power output
$$P_0 = I^2 R_L$$
 conversion efficiency $\eta = \frac{P_0}{Q_H}$

here
$$I = \frac{\alpha_{p1}(T_h - T_{p1}) + \alpha_{p2}(T_{p2} - T_c) - \alpha_{n1}(T_h - T_{n1}) - \alpha_{n2}(T_{n2} - T_c)}{R_{in} + R_L}$$

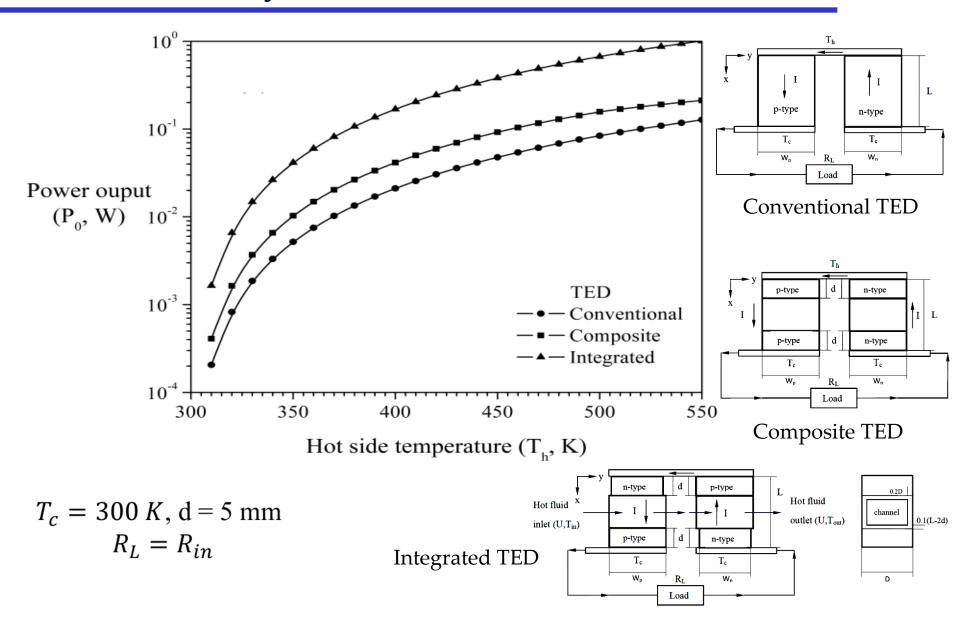
$$R_{in} = \frac{\rho_{n1}d + \rho_{cn}(L - 2d) + \rho_{n2}d}{A_n} + \frac{\rho_{p1}d + \rho_{cp}(L - 2d) + \rho_{p2}d}{A_p}$$

where
$$A_n = W_n \times D$$
 and $A_p = W_p \times D$

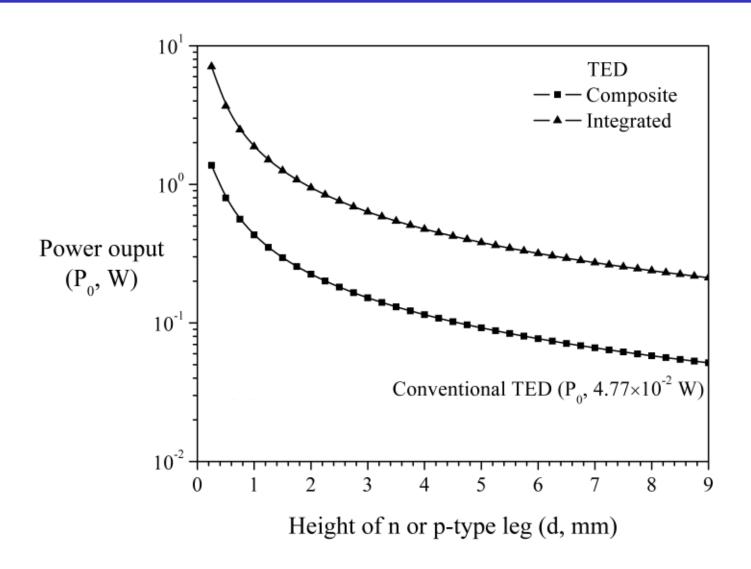
To achieve $\eta_{max'}$ an optimized width of p-type material is

$$W_{p} = W_{n} \left[\frac{\left((\rho_{p1} + \rho_{p2})d + \rho_{c}(L - 2d) \right) \left(\frac{1}{\frac{d}{Lk_{n1}} + \frac{L - 2d}{Lk_{c}} + \frac{d}{Lk_{n2}}} \right)}{\left((\rho_{n1} + \rho_{n2})d + \rho_{c}(L - 2d) \right) \left(\frac{1}{\frac{d}{Lk_{n1}} + \frac{L - 2d}{Lk_{c}} + \frac{d}{Lk_{n2}}} \right)} \right]^{1/2}$$

CTED-Analytical Results



CTED-Analytical Results

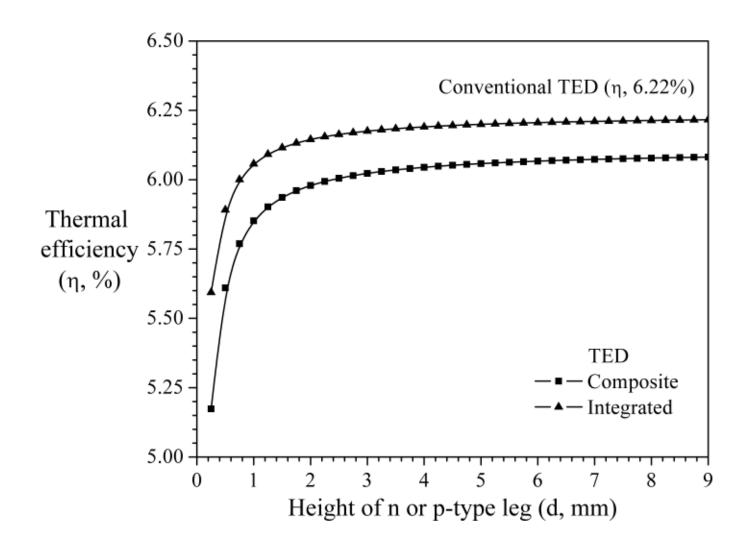


$$T_c = 300 K$$

$$T_h = 450 K$$

$$R_L = R_{in}$$

CTED-Analytical Results



$$T_c = 300 K$$

$$T_h = 450 K$$

$$R_L = R_{in}$$

CTED-Figure of Merit

 The modified Figure of Merit equation with the following geometric equivalent relations:

$$P_0 = I^2 R_L$$

Equivalent Electrical Resistance:

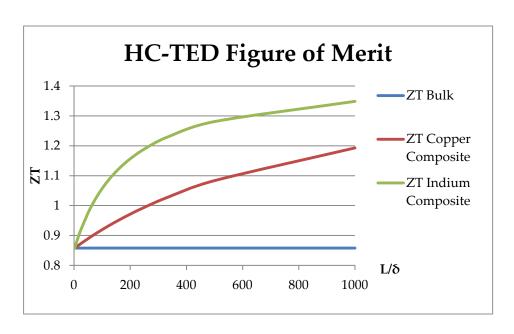
$$\rho^* = \frac{\rho_{SC} 2\delta}{L} + \frac{\rho_C (L - 2\delta)}{L}$$

• Using two intermediate materials of Copper or Indium, the $Z\overline{T}$ is calculated based on the ratio of L/δ with constant material properties:

$$\eta=rac{P_0}{Q_H}$$

CTED-ZT

Redefining ZT to include N-type Bi₂(Te,Se)₃ layers with material properties evaluated average temperature



δ [mm]	ZT(In)	ZT(Cu)
1	0.863	0.881
0.1	0.919	1.057
0.01	1.192	1.348
0.001	1.450	1.430
0.000 1	1.500	1.440
0.000 01	1.505	1.441

*Based upon L = 10 [mm]

As $L/\delta \rightarrow \infty$, for In – composite,

$$Z\bar{T}_{conv} = 0.858$$

$$Z\bar{T}_{comp,In} = 1.686$$

96% increase!

TEDs- Numerical Solutions

Governing equations

Fluid domain:

$$\nabla \cdot \mathbf{v} = 0 \tag{1}$$

$$\rho_f.(\mathbf{v}\nabla\mathbf{v}) = \nabla P + \mu \nabla^2 \mathbf{v}$$
 (2)

$$(\rho c)_f (\mathbf{v} \nabla T) = \nabla \cdot (k_f \nabla T)$$
(3)

Thermoelectric material:

$$\nabla . \mathbf{J} = 0$$
 Thomson effect (4)

$$\nabla . \mathbf{J} = 0 \qquad \text{Thomson effect}$$

$$\nabla (k \nabla T) + \rho \mathbf{J}^{2} - T \mathbf{J} \cdot \left[\left(\frac{\partial \alpha}{\partial T} \right) \nabla T + (\nabla \alpha)_{T} \right] = 0$$
(5)

Joule heating

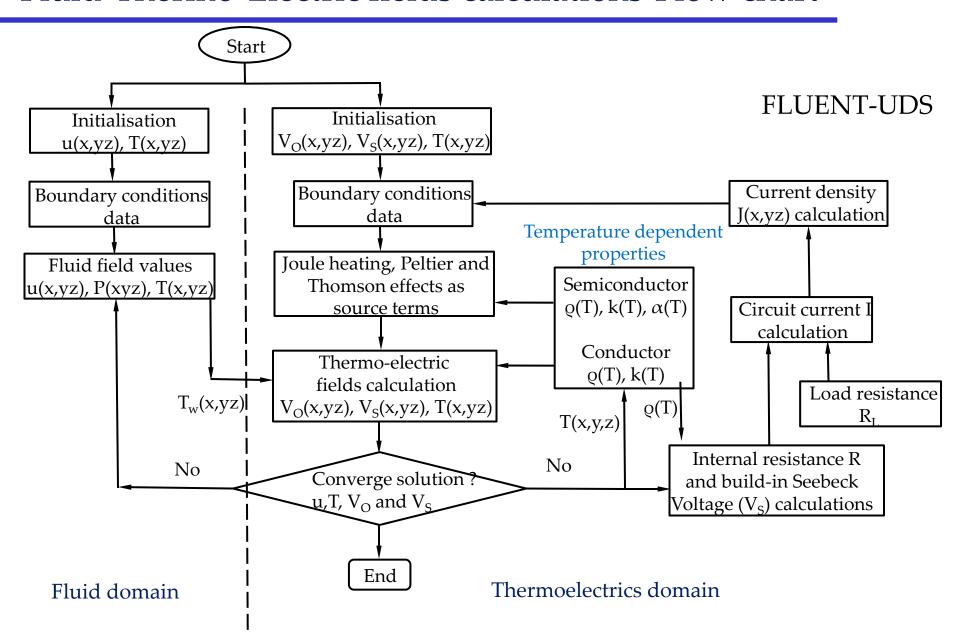
$$\nabla V = \nabla V_{OEMF} + \nabla V_{SEMF} = -\rho \mathbf{J} - \alpha \nabla T$$

$$\uparrow \qquad \uparrow \qquad \uparrow \qquad (6)$$

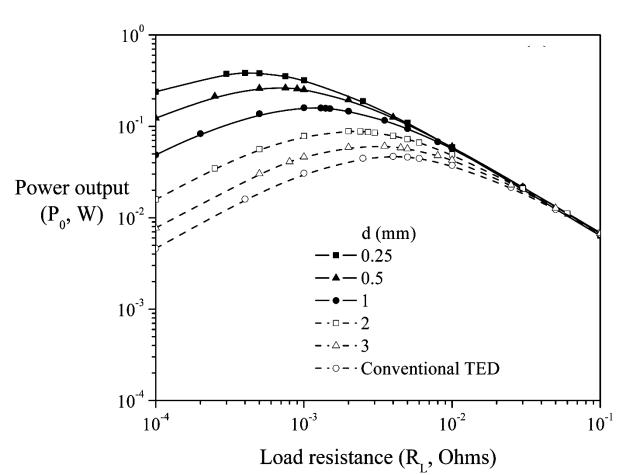
Electrostatic distribution

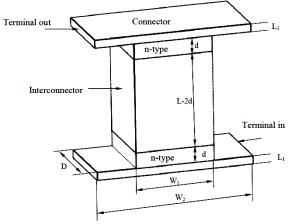
Seebeck voltage distribution

Fluid-Thermo-Electric fields calculations-Flow chart



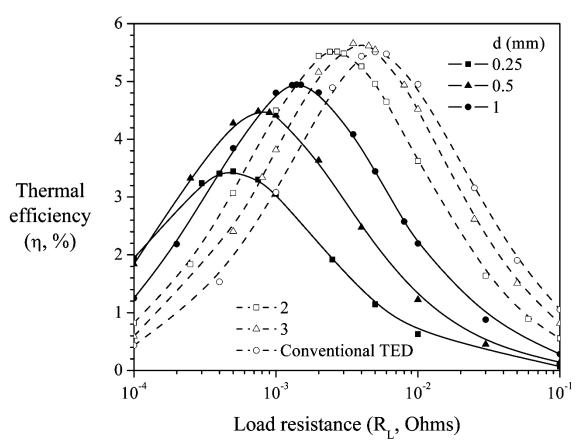
CTED- Power output

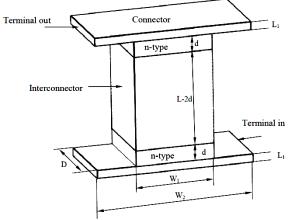




$$T_c = 300 K$$
$$T_h = 450 K$$

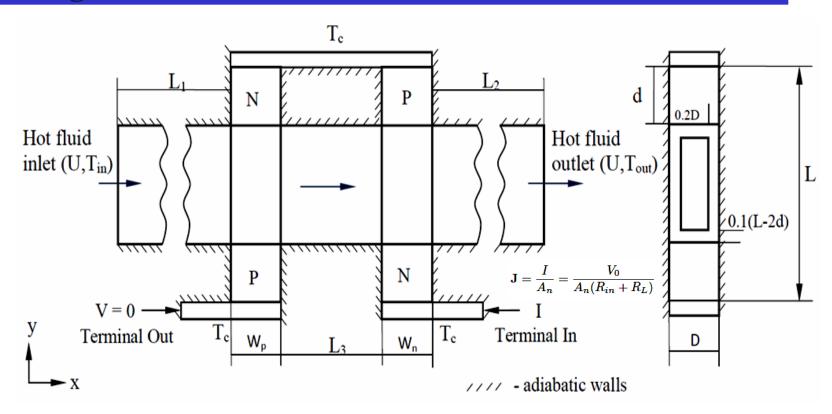
CTED- Conversion efficiency





$$T_c = 300 K$$
$$T_h = 450 K$$

Integrated TED



Thermoelectric materials:

Homogeneous , isotropic Temperature dependent properties $\varrho(T),\,k(T)\text{ and }\alpha(T)$ Thermo-electrical interface contact resistances are negligible n-type (75% Bi₂Te₃, 25% Bi₂Se₃)

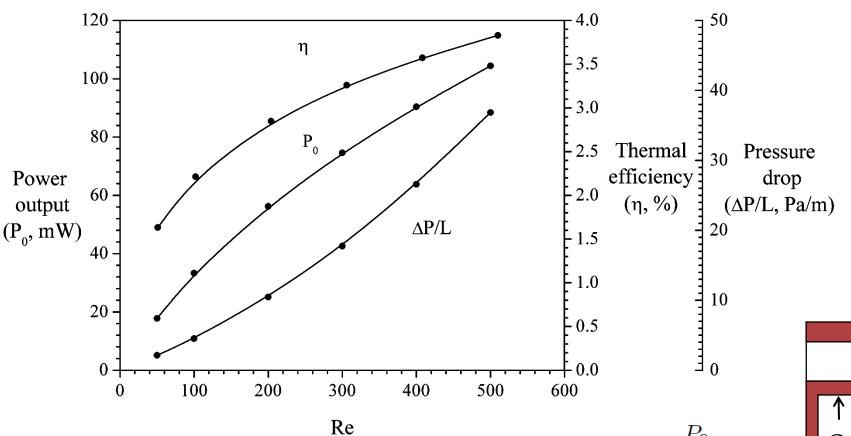
p-type (25% Bi₂Te₃, 75%Sb₂Te₃, 1.75 excess Se)

Fluid-Air

Flow:

Steady, laminar and incompressible flow

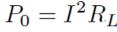
iTED- Flow rate (Re)



$$T_{in} = 550 \text{ K}$$
, $T_c = 300 \text{ K}$, $d = 5 \text{ mm}$, $R_{in} = R_L$

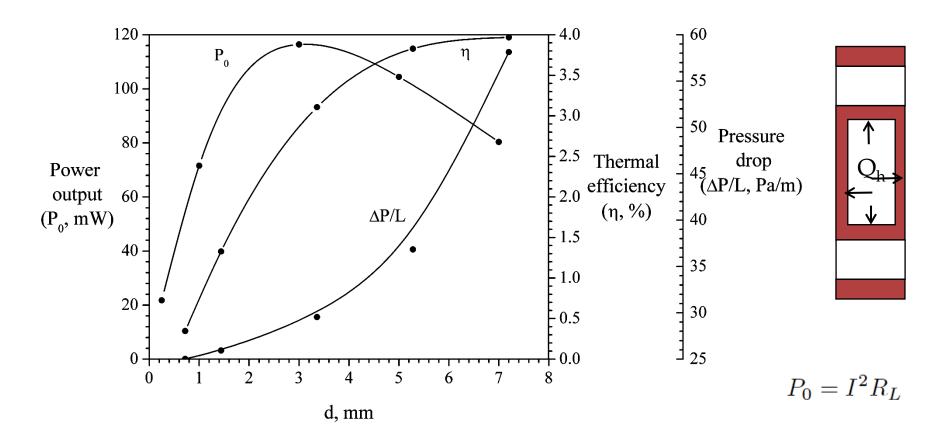
$$Q_h$$

$$P_0 = I^2 R_L$$





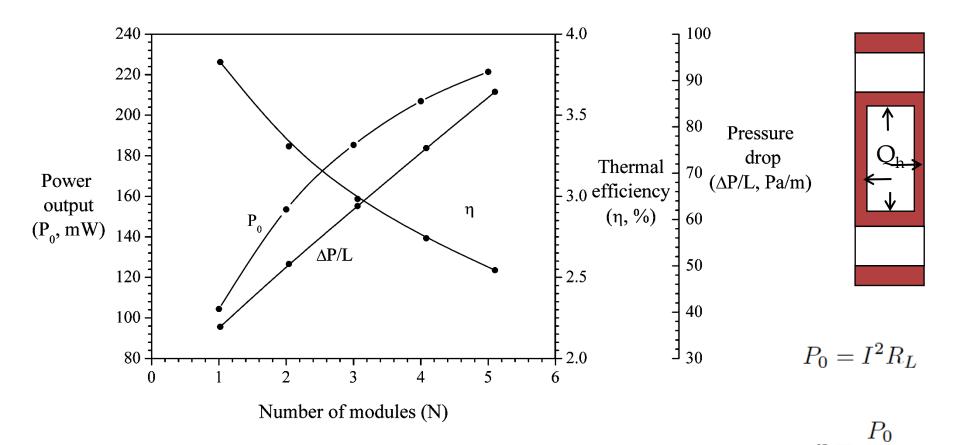
iTED- Semiconductor slice size (d)

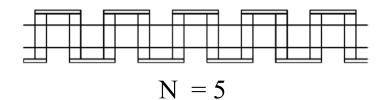


Re = 500,
$$T_{in}$$
 = 550 K, T_{c} = 300 K, R_{in} = R_{L}

$$\eta = \frac{P_0}{Q_h}$$

iTED- Number of modules (N)





$$Re = 500$$
, $T_{in} = 550$ K, $T_{c} = 300$ K, $R_{in} = R_{L}$

Conclusions

- Using analytical solutions, It is demonstrated that the iTED and CTED show nearly an eight-fold and four-fold increase in both power output and heat input respectively, when compared to the conventional TED values.
- Analytically derived $Z\overline{T}$ for composite –TED (with In as inserted metal, similar for Cu) has a limiting value of 1.686 for L/ $\delta \rightarrow \infty$, compared to 0.858 for the corresponding conventional TED
- The semiconductor slice size laminated on inter-connector has substantial influence on both CTEDs and iTEDs performance.
- iTED design with rearranged p-n configuration, alleviates heat flowback problem and heat transfer increase strongly with flow rate and number of modules.
- CTEDs and iTEDs capable of extracting large amounts of available waste heat from automobile exhaust gases, power plants and industrial processes where the conversion efficiency TED alone is not on priority.