# Numerical modelling of the performance of thermoelectric elements

Knud Zabrocki[1], P. Ziolkowski[1], R. Sottong[1], and Eckhard Müller[1,2]

## Classical thermal energy balance equation for thermoelectric devices

### Introduction

- Performance of thermoelectric devices – in the framework of continuum theory
- TE effects - interference of two irreversible processes: Heat transport and charge carrier transport
- Onsager-de Groot-Callen theory: Thermoelectrics as a kind of „field theory " in non-equilibrium thermodynamics
- Description via differential equations - thermal energy balance equation

Lars Onsager * 27.11.1903; †05.10.1976
Sybren Ruurds de Groot * 18.04.1916; †09.05.1994
Herbert B. Callen * 1919; †22.05.1993

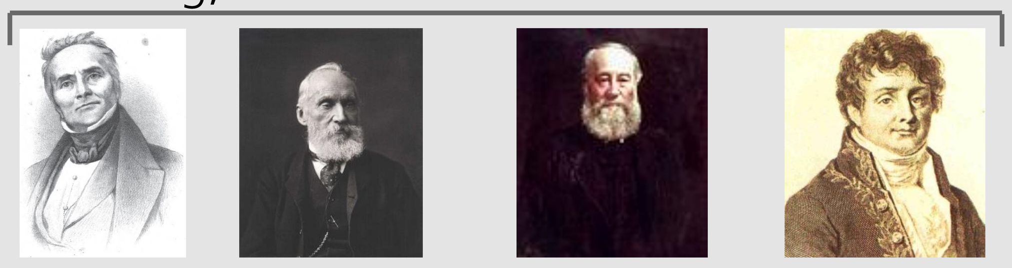
**Fig. 1 Influential personalities in macroscopic theory of thermoelectricity – Onsager – de Groot – Callen**

### Thermal energy balance

- Coupling of Fourier's and Ohm's law
- Transport coefficients - Onsager relations
- Local energy balance $\varrho_d c \frac{\partial T}{\partial t} + \nabla \cdot \dot{\mathbf{q}} = \mathbf{j} \cdot \mathbf{E}$
- Heat flux: $\dot{\mathbf{q}} = -\kappa_j \nabla T + \boldsymbol{j}\, \alpha\, T$
- Divergence of the heat flux different terms

$$\nabla \cdot \dot{\mathbf{q}} = \tau\, \mathbf{j} \cdot \nabla T + \mathbf{j} \cdot \mathbf{E} - \frac{\boldsymbol{j}^2}{\sigma_T} - \nabla \cdot (\kappa_j \nabla T)$$

- Representing Peltier, Thomson effects, Joule heating, Fourier heat conduction



J. C. A. Peltier * 22.02.1785; † 27.10.1845
William Thomson Lord Kelvin * 26.06.1824; †17.12.1907
J. P. Joule * 24.12.1818 †11.10 1889
J. B. J. Fourier * 21.3.1768- † 16.5.1830)

**Fig. 2 Scientists - Non-equilibrium Thermodynamics**

### Performance of a TE element

- Performance depends on:
  - Temperature-dependent material properties
  - Working/boundary conditions (BC) like junction temperatures and heat fluxes, load resistance, electrical current
  - Contact quality (resistance)
  - Coupling to the surrounding (convection, radiation)
  - Geometry/shape of the TE elements

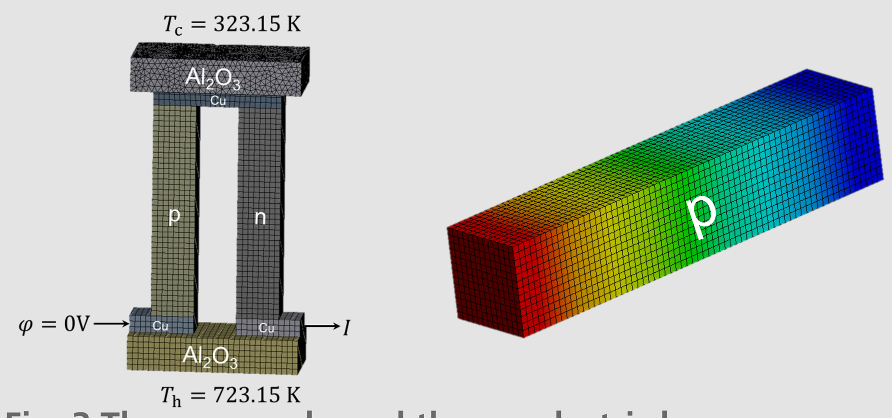



**Fig. 3 Thermocouple and thermoelectric leg**

## Numerical modelling of the performance of thermoelectric elements

### Numerical methods

- TE phenomena on macroscopic scale (Characteristic time and length scales $\tau \geq 10^{-3}$ s and $l \geq 10^{-3}$ m) – description via non-linear differential equations with state-dependent coefficients
- No analytic solution for heat balance → classical numerical methods
  - *Finite difference method*
  - *Finite element method*
  - Finite Volume method
- Finite difference method: the simplest and most straightforward interpolation method, best studied and established
- Euler method: differential coefficient to difference coefficient, iterative method
- boundary value problem to initial value problem: shooting method

### Example calculation for a TE element

- Measured temperature dependence of material data (discontinuous) → fitting or interpolation (continuous)

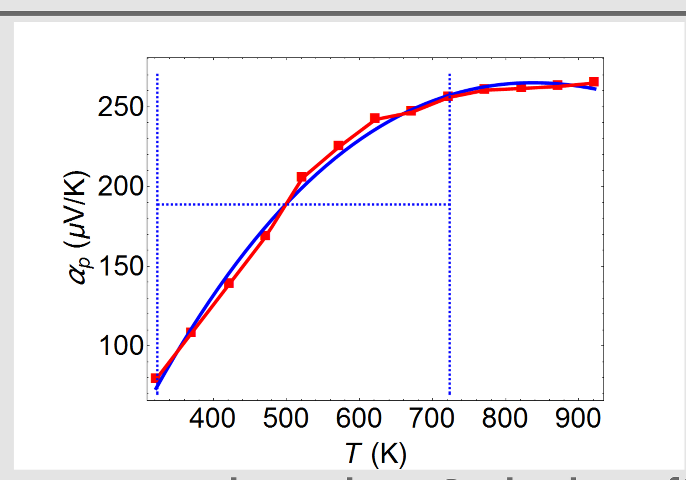



**Fig. 4: Temperature dependent Seebeck coefficient; Red points – measurement, red line – linear interpolation, blue line – fit, blue dashed line - average**

- Temperature averages for using constant properties model for analytical solutions

| $\bar{\kappa}$ [W/(m · K)] | $\bar{\varrho}$ [Ω · m] | $\bar{\alpha}$ [µV/K] | $f = \bar{\alpha}^2/\bar{\varrho}$ [W/(m · K²)] | $zT_m$ |
|---|---|---|---|---|
| 1.46885 | $1.37742 \cdot 10^{-5}$ | 188.719 | $2.58562 \cdot 10^{-3}$ | 0.921 |

**Tab 1: Example – averaged material properties**

### Numerical results compared with CPM

- Temperature profiles and performance

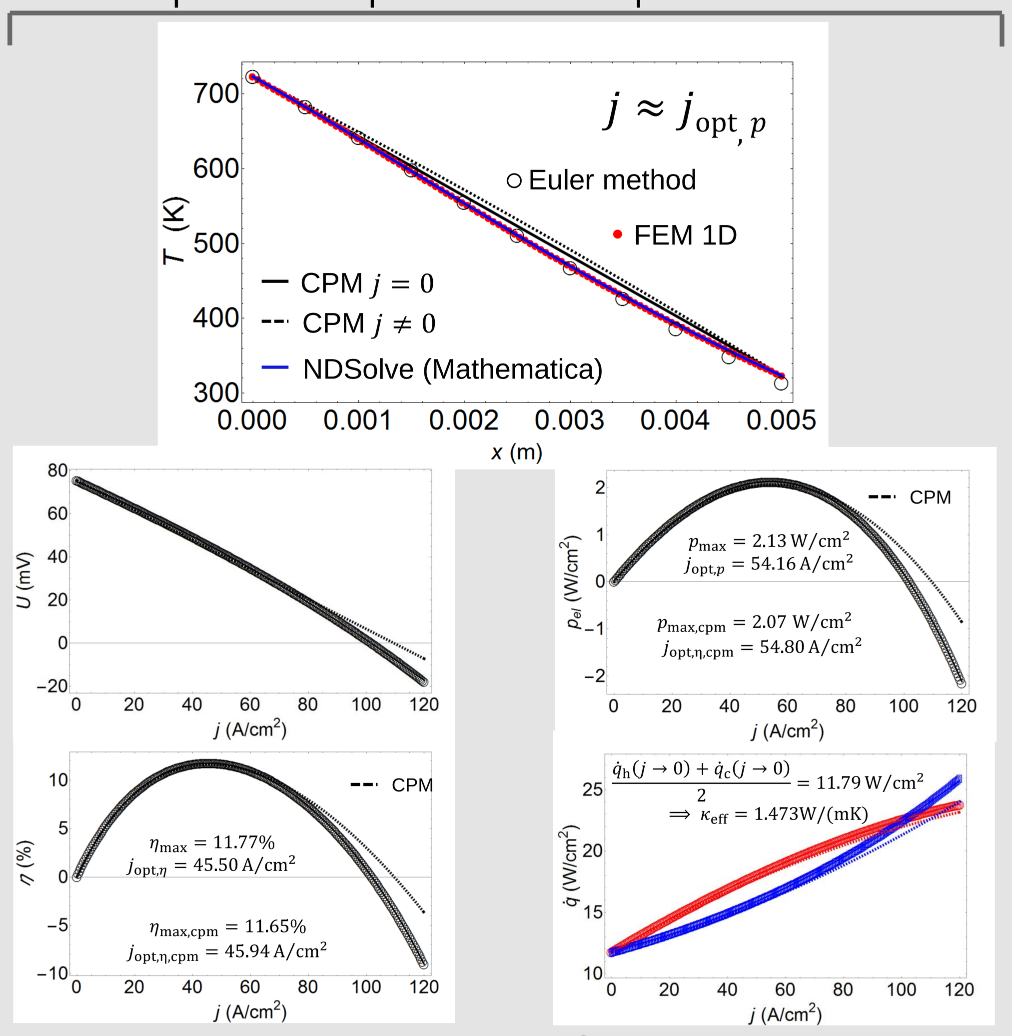



**Fig. 5: FDM/CPM calculation of the p-type element**

## Finite element method – Performance calculations

### FEM simulation

- Real 3D geometry - TEG design – different layers, variation of thickness, spacing, filling factors
- Fluid-Solid coupling (CFD-FEM), heat exchanger design, coupling to a system
- Combination of temperature dependence of material properties and contact resistances
- Current carrying capacity of the connections
- Shaped, anisotropic, segmented elements

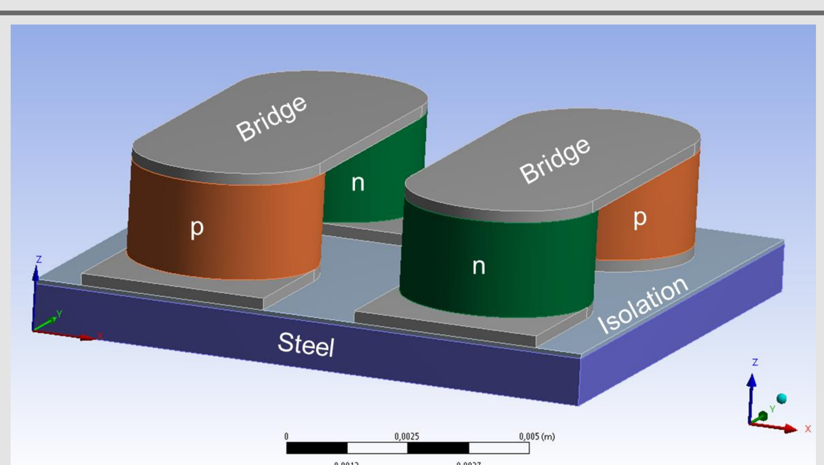



**Fig.7: Two connected pn-TE couples.**

### Constant temperature operation

- Constant boundary temperatures ⇒ spatial distribution of the heat flux – Integration

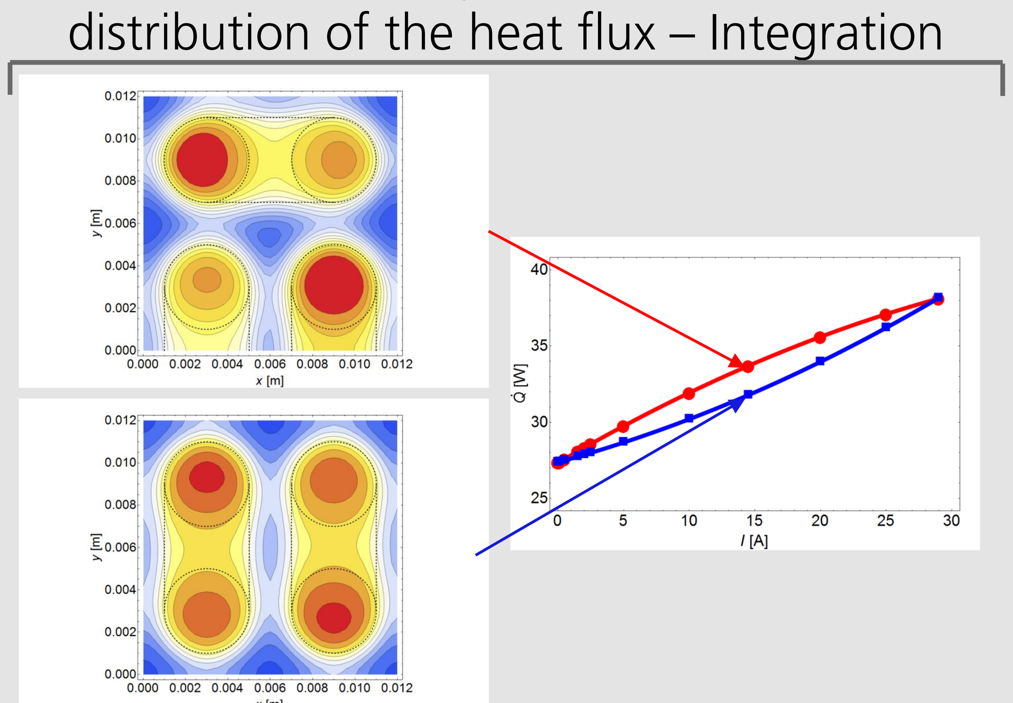


**Fig. 8: Heat flux hot side (above) – cold side (below).**

- For every current point

$$\vec{j}_Q = \vec{j}_Q(x,y) \;\Rightarrow \dot{Q} = \iint \vec{j}_Q(x,y)\,\mathrm{d}x\mathrm{d}y$$

- Efficiency and Power optimization at different electrical currents

### Constant heat input operation

- Fixed heat flow at the hot side $\dot{Q}_h$ and $T_c$
- Constant heat flow ⇒ spatial distribution of the hot side temperature
- Variation of hot side temperature with the current *I*

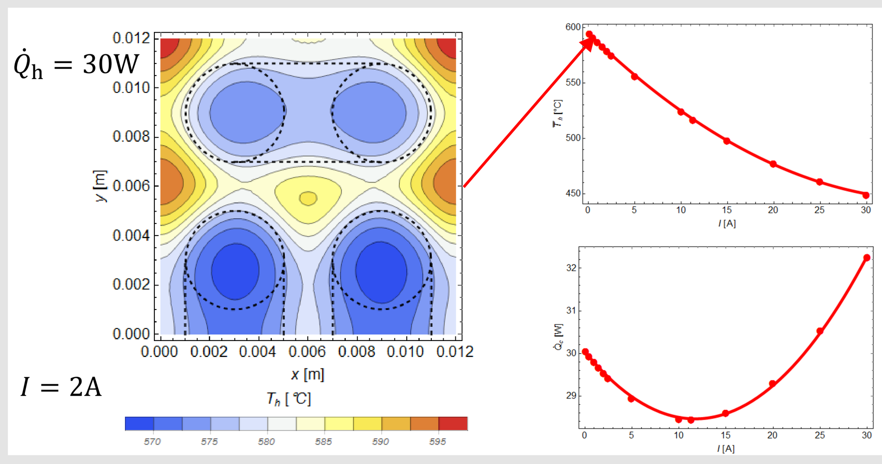
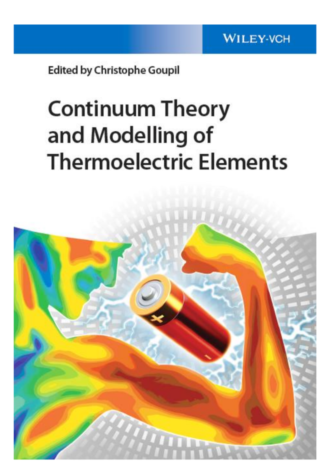



**Fig. 9: Hot side temperature and cold side heat**

- Power output and efficiency optimized at same current

**Affiliations**
[1]Institute of Materials Research, German Aerospace Center (DLR), D-51170 Köln, Germany
[2]JLU Giessen, Institute of Inorganic and Analytical Chemistry, 35392 Giessen, Germany

**Details in Chapter 6 of "Continuum Theory and Modelling of Thermoelectric Elements", Release date Feb. 2016**




Deutsches Zentrum für Luft- und Raumfahrt

**Contact**
German Aerospace Center
Institute of Materials Research
51147 Cologne
Germany
Knud.Zabrocki@dlr.de
+49 (0) 2203/601-3359