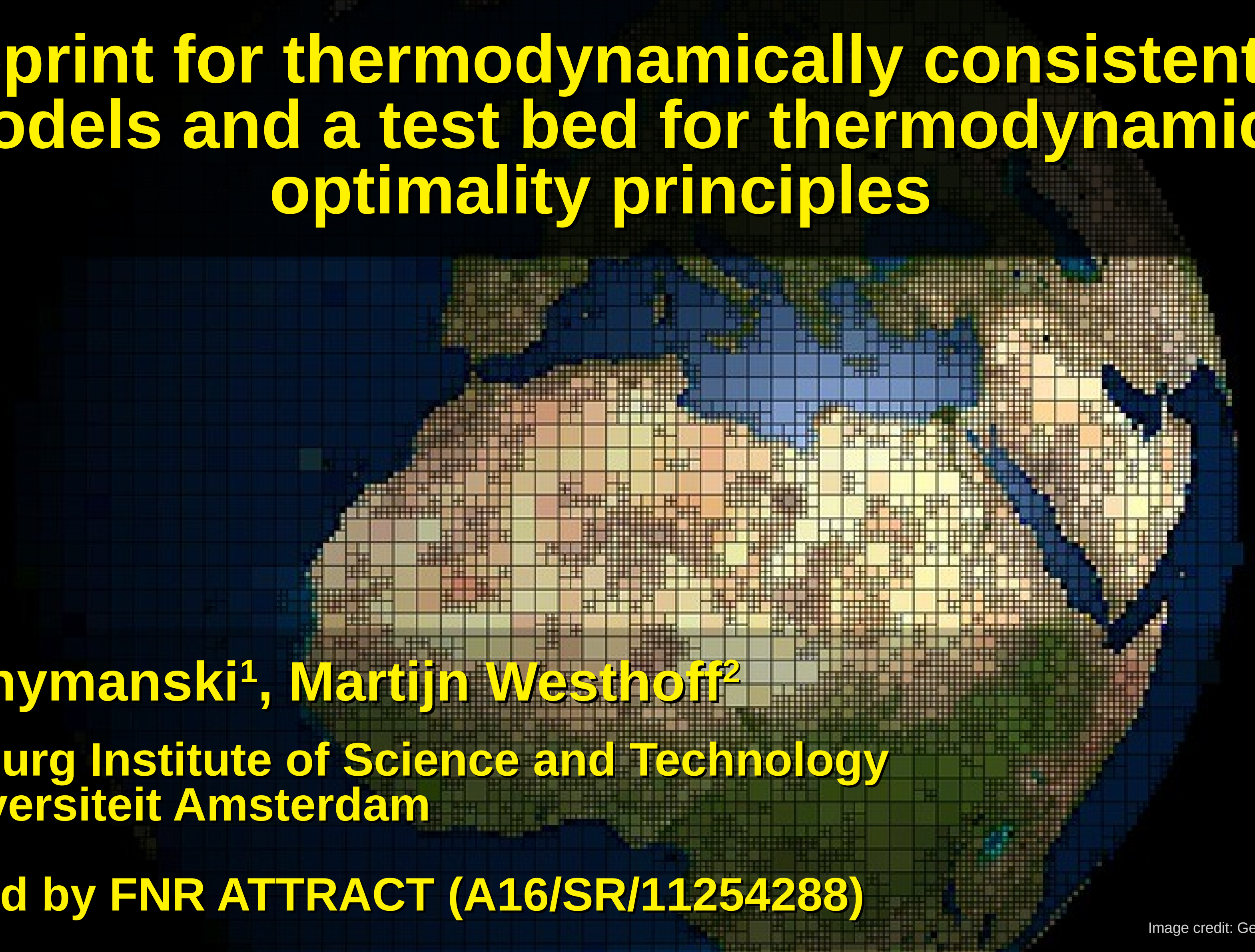
A blueprint for thermodynamically consistent box models and a test bed for thermodynamic optimality principles



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[1]Luxembourg Institute of Science and Technology
[2]Vrije Universiteit Amsterdam

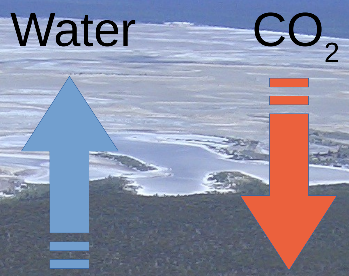
[1]Supported by FNR ATTRACT (A16/SR/11254288)

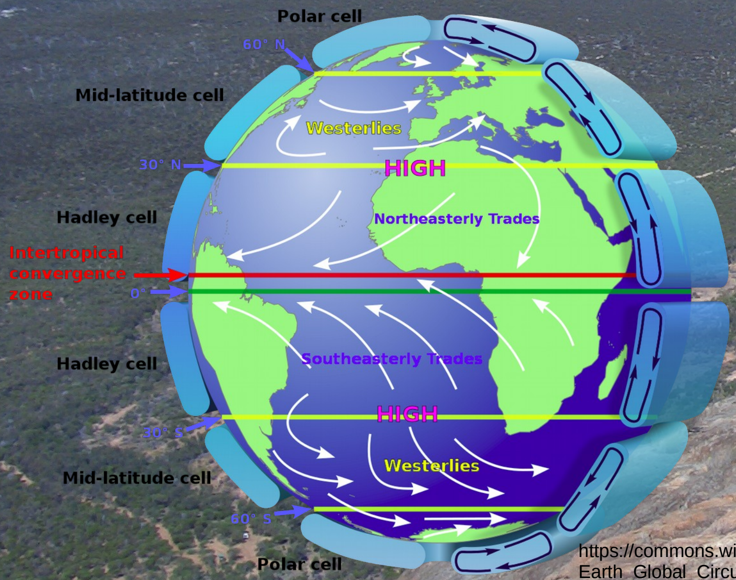
Image credit: Gerd Altmann, pixabay.com

MOTIVATION FOR THERMODYNAMIC OPTIMALITY:

HOW CAN WE UNDERSTAND

1. THE BEHAVIOUR OF ECOSYSTEMS?
2. ATMOSPHERIC HEAT TRANSPORT PATTERNS?





https://commons.wikimedia.org/wiki/File:Earth_Global_Circulation_-_en.svg

Image: Peak Charles NP, by Stan Schymanski

ODUM & PINKERTON (1955): MAXIMUM POWER (MEP → MP)

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TIME'S SPEED REGULATOR: THE OPTIMUM EFFICIENCY FOR MAXIMUM POWER OUTPUT IN PHYSICAL AND BIOLOGICAL SYSTEMS

By HOWARD T. ODUM[1] and RICHARD C. PINKERTON

University of Florida, Gainesville

American Scientist 43(2), (1955)

"What has been lacking, however, is a generalization applicable to open systems which would indicate the rate of entropy increase."

"Our proposition is that natural systems tend to operate at that efficiency which produces a maximum power output."

"...to operate at maximum power, the efficiency may never exceed 50 per cent of the ideal "reversible" efficiency."

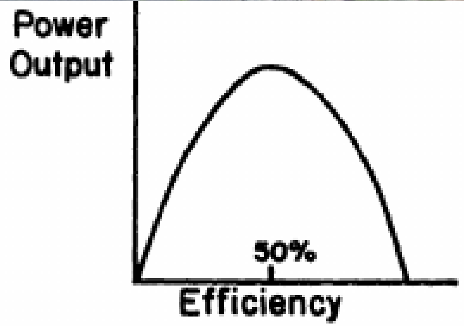


FIG. 2. Power output is given as a function of efficiency for systems where there is no leakage (l) and the efficiency (E) is thus equal to the force ratio (R).

GARTH PALTRIDGE (1978): MAXIMUM ENTROPY PRODUCTION (MEP)

23 years after Odum and Pinker, Paltridge independently proposed the maximum entropy production principle to explain global climate patterns...

Quart. J. R. Met. Soc. (1978), 104, pp. 927–945

551.513.1:551.58

The steady-state format of global climate

By G. W. PALTRIDGE

CSIRO, Division of Atmospheric Physics, Mordialloc, Victoria 3195, Australia

"the earth-atmosphere system obeys a basic extremum principle of maximum dissipation or entropy production."

KLEIDON (2010): "MP EQUIVALENT TO MEP"

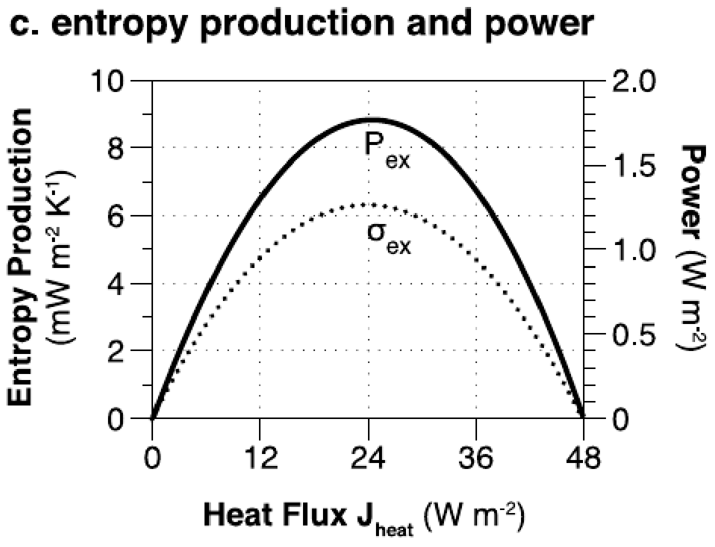
Another 30 year later, back from maximum entropy production (MEP) to the maximum power (MP) principle. Axel Kleidon: MP mostly the same as MEP

ELSEVIER
Physics of Life Reviews 7 (2010) 424–460
www.elsevier.com/locate/plrev

Review

Life, hierarchy, and the thermodynamic machinery of planet Earth

Axel Kleidon



Same 50% rule as 60 year earlier!

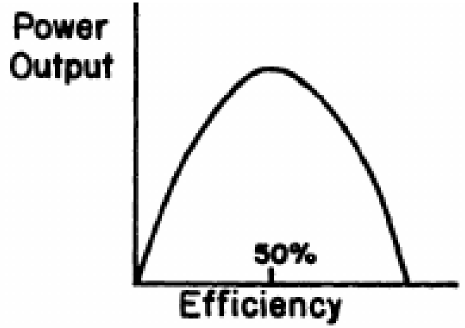


FIG. 2. Power output is given as a function of efficiency for systems where there is no leakage (l) and the efficiency (E) is thus equal to the force ratio (R).

Odum & Pinkerton (1955)

CARNOT LIMIT FOR MAXIMUM POWER

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Explicit system drawings help understand MEP vs. MP:

- Heat injected into hot reservoir (J_{oh}) and removed from cold reservoir (J_{co}).
- Spontaneous heat flow from hot to cold → entropy production (σ) and allows power extraction (*G*).
- **Carnot limit: maximum extractable power when σ=0**

Motivation

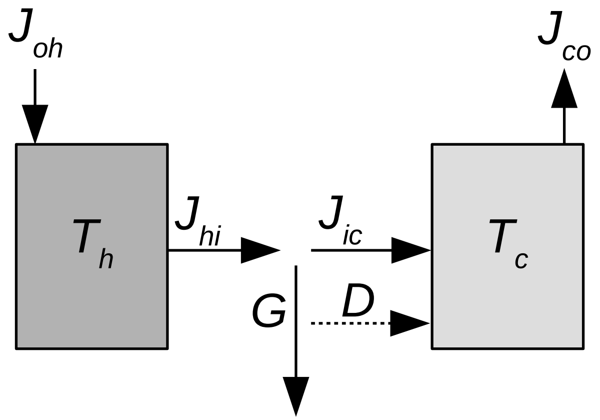
MP vs. MEP

Drawings

Blueprint

Examples

Conclusions



Energy balance:

$J_{co} = J_{ic}$

$J_{ic} = J_{hi} - G$

$J_{hi} = J_{oh}$

$$\sigma = \frac{J_{ic}}{T_c} - \frac{J_{hi}}{T_h}$$

Set σ = 0, substitute J_{ic} and solve for G

$$G_{max} = J_{hi}\frac{(T_h - T_c)}{T_h}$$

Carnot-limit

ROLE OF DISSIPATED POWER

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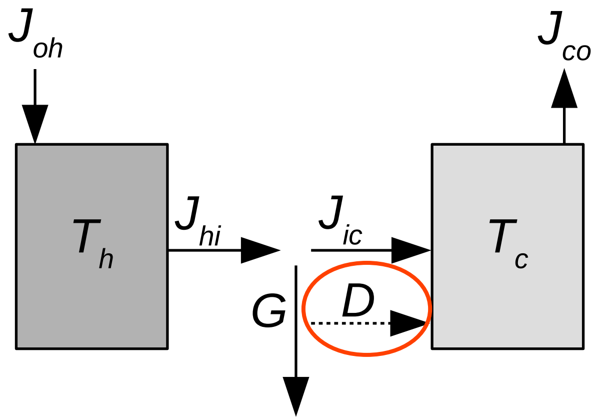
- Part of power often assumed to be dissipated (converted to heat, *D*) by the heat engine and transferred to cold res.
- D needs to be considered in energy and entropy balance
- How will it affect the Carnot limit?

Energy balance:

$J_{co} = J_{ic} + D$
$J_{ic} = J_{hi} - G$
$J_{hi} = J_{oh}$



$$\sigma = \frac{J_{ic}}{T_c} - \frac{J_{hi}}{T_h} + \frac{D}{T_c}$$

Set σ = 0, substitute J_{ic} and solve for G

$$G_{max} = J_{hi}\frac{(T_h - T_c)}{T_h} + D$$

But it is absurd: the greater the dissipation, the more G we could extract.
→ **Perpetual motion!**

BEJAN (2016):
ENGINE & BREAK SYSTEM

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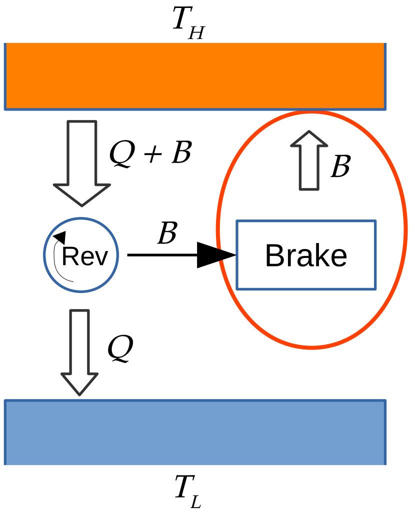
Similar potential for confusion in book by A. Bejan!

Bejan (2016):
"The more irreversible the operation of the engine, the less power remains on its shaft, to be dissipated in the brake."



Schymanski and Westhoff:
"But a brake pumping heat back into the hot reservoir could result in ***perpetual motion!****"*

"Figure 3.16 Destruction of useful work in the "temperature gap system" traversed by a heat current."

Redrawn after Figure 3.16 c in: Bejan, A.: Advanced engineering thermodynamics, Fourth edition., John Wiley & Sons Inc, Hoboken, New Jersey, 2016.

HOW TO RESOLVE CONFUSION ABOUT POWER AND DISSIPATION?

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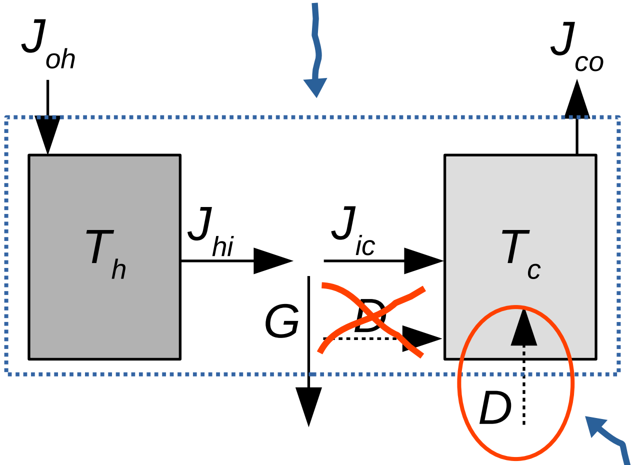
"Power" is transport of free energy across a boundary. Need to draw such a boundary:



Energy balance:

$$J_{co} = J_{ic} + D$$
$$J_{ic} = J_{hi} - G$$
$$J_{hi} = J_{oh}$$

$$\sigma = \left(\frac{J_{out}}{T_c} - \frac{J_{in}}{T_h}\right) \geq 0 \quad \rightarrow \quad \sigma = \frac{J_{ic}}{T_c} - \frac{J_{hi}}{T_h} + \frac{D}{T_c}$$

$$G_{max} = J_{hi}\frac{(T_h - T_c)}{T_h} + D$$

Now it becomes clear that the dissipation has to happen in the same place where the power went!

So dissipation happens outside of the system if power was extracted across the boundary, and if we add the heat back to the cold reservoir, it is an external entropy flux, not internal entropy production.

NEW BLUEPRINT FOR SELF-CONSISTENT BOX MODELS USING OPEN SOURCE TOOLS

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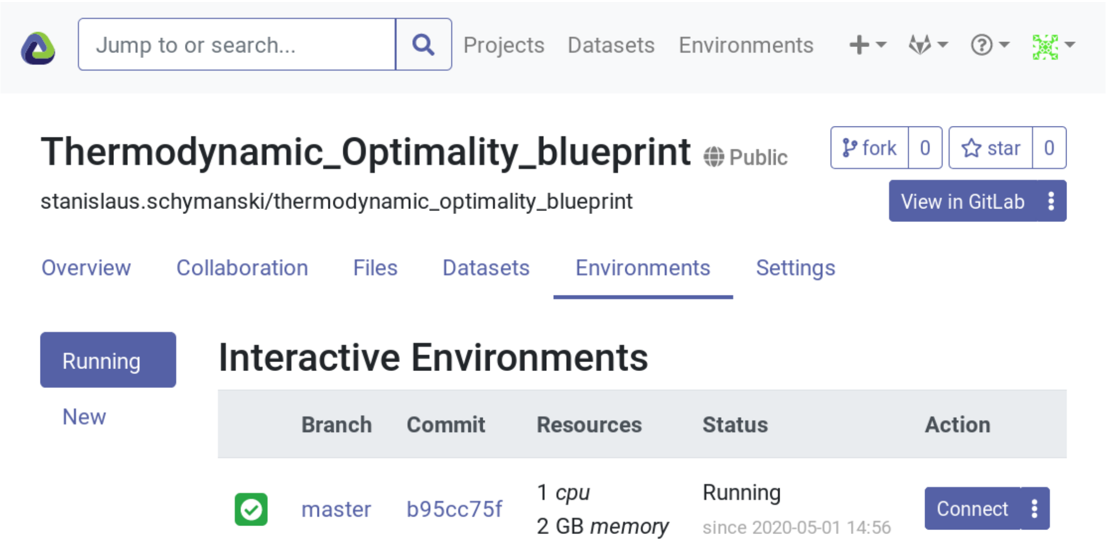
To avoid such misunderstandings, I developed a blueprint for self-consistent box models, which is exclusively based on open source software, such as python, jupyter and the python packages SymPy and ESSM. In the following, we will explain the systematic approach while showing screenshots from jupyter notebooks available here: https://renkulab.io/projects/stanislaus.schymanski/thermodynamic_optimality_blueprint
All derivations and data can be reproduced online and adjusted to your liking at the above link!



1. DRAW ALL RELEVANT FLUXES AND SYSTEM BOUNDARIES

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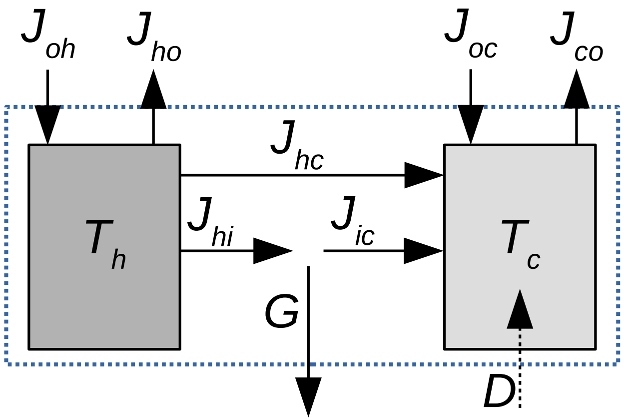
First of all, we need to create a drawing with clear system and sub-system boundaries and fluxes.



2. FORMULATE ENERGY BALANCE CLOSURE

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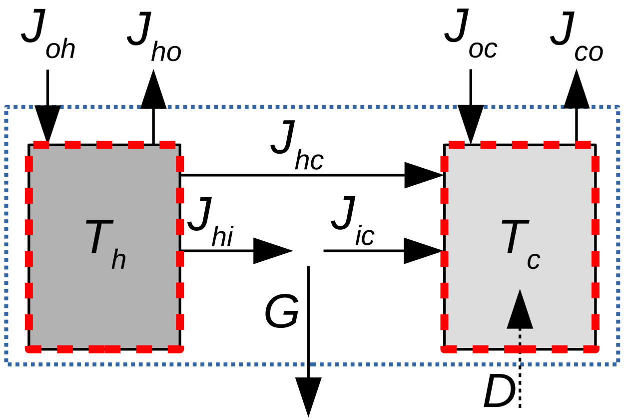
Now, we can define energy balance equations for each sub-system individually and for the whole system. Note that the extracted power removes energy from that flux, such that the energy leaving the hot system is less than the energy reaching the cold system.



3.2 Energy balance

At steady state, the incoming and outgoing fluxes for each reservoir have to match.

```
class eq_energy_h(Equation):
    """Steady state energy balance for hot reservoir."""

    expr = Eq(0, J_oh - J_ho - J_hc - J_hi)
display(eq_energy_h)

class eq_energy_c(Equation):
    """Steady state energy balance for cold reservoir."""

    expr = Eq(0, J_hc + J_ic + J_oc + D - J_co)
display(eq_energy_c)
```

$$0 = -J_{hc} - J_{hi} - J_{ho} + J_{oh}$$

$$0 = D - J_{co} + J_{hc} + J_{ic} + J_{oc}$$

3. DEFINE FLUXES AND THEIR DRIVERS

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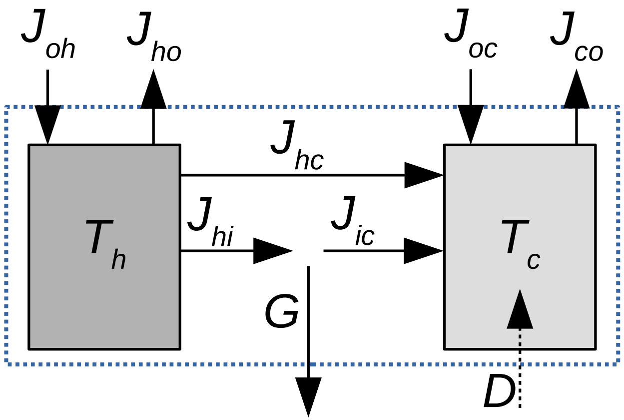
Define equations for the relevant fluxes as a function of their drivers, e.g. the heat transfer from the hot to the cold box as a function of the temperature difference etc. Here we use linear equations, e.g. for blackbody radiation (J_{co})




```
class eq_Jco(Equation):
    """J_co as a function of T_c"""
    expr = Eq(J_co, k_co * T_c)
display(eq_Jco)

class eq_D(Equation):
    """D as a fraction of G."""
    expr = Eq(D, k_D * G)
display(eq_D)
```

$$J_{ho} = T_h k_{ho}$$

$$J_{hi} = k_{hi} \left(-T_c + T_h\right)$$

$$J_{hc} = k_{hc} \left(-T_c + T_h\right)$$

$$J_{ic} = -G + J_{hi}$$

$$J_{co} = T_c k_{co}$$

$$D = G k_D$$

4. IDENTIFY KNOWNS AND UNKNOWNS AND SOLVE FOR STEADY STATE

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Now we choose the knowns and unknowns, and solve the system of equations for the unknowns (here 8 equations and 8 unknowns). Using sympy, this can be done automatically and we get analytical solutions without doing any of the maths ourselves. Transparent, verifiable and reproducible!

Motivation

MP vs. MEP

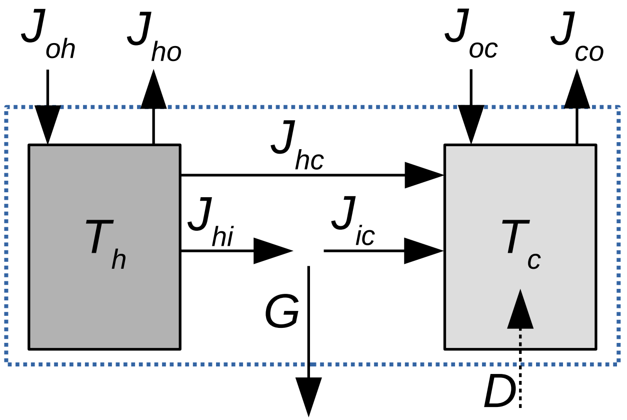
Drawings

Blueprint

Examples

Conclusions

Solve system of equations for steady-state:




```
[8]: list_eqs = [eq_Jho, eq_Jhi, eq_Jhc, eq_Jic, eq_Jco, eq_D, eq_energy_h, eq_er
     soln = solve(list_eqs, J_ho, J_hi, J_hc, J_ic, J_co,
                  D, T_c, T_h)
     soln
```

[8]: $\Big\{ D : Gk_D, \ J_{co} : \frac{k_{co}\left(Gk_D\left(k_{hc}+k_{hi}+k_{ho}\right) - G\left(k_{hc}+k_{hi}+k_{ho}\right) + J_{oc}\left(k_{hc}+k_{hi}+k\right.\right.}{k_{co}k_{hc}+k_{co}k_{hi}+k_{co}k_{ho}+k_{hc}k_{ho}+k_{hi}k_{ho}}$

$: \frac{-Gk_Dk_{hi}k_{ho} - G\left(k_{co}k_{hc}+k_{co}k_{hi}+k_{co}k_{ho}+k_{hc}k_{ho}\right) - J_{oc}k_{hi}k_{ho} + J_{oh}k_{co}k_{hi}}{k_{co}k_{hc}+k_{co}k_{hi}+k_{co}k_{ho}+k_{hc}k_{ho}+k_{hi}k_{ho}}, \ T_c :$

Equations to compute internal fluxes and temperatures for given transfer coefficients and boundary fluxes

WHAT HAPPENS TO TEMPERATURES AS I EXTRACT MORE POWER?

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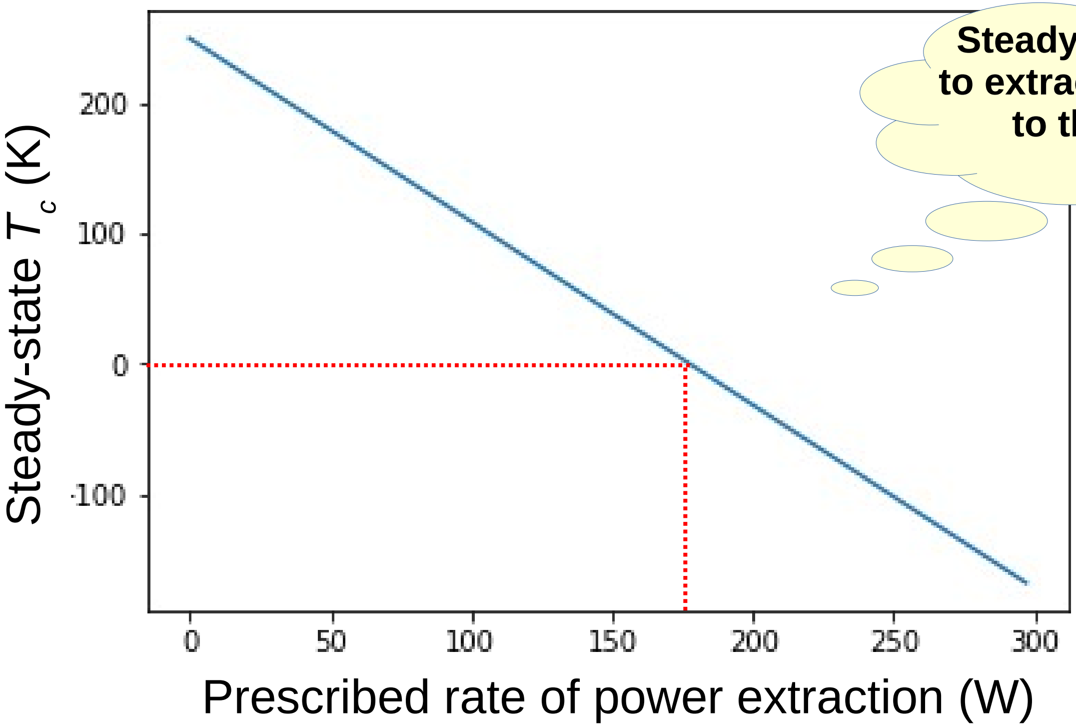
```
vdict = {}
vdict[J_oh] = 300.
vdict[J_oc] = 1.
vdict[k_ho] = 0.7
for const1 in [k_hc, k_D, D]: vdict[const1] = 0
vdict[k_hi] = 1.
vdict[k_co] = 0.3
dict_forcing = vdict.copy()
```



Steady-state solution allows us to extract work without end, even to the point that T_c would become negative.

Missing constraint: entropy balance!

5. DEFINE ENTROPY EXCHANGE AND PRODUCTION TERMS

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Entropy exchange vs. entropy production

Heat flux out removes entropy (e.g. J_{ho}/T_h).
Heat flux in adds entropy (e.g. J_{oh}/T_h).

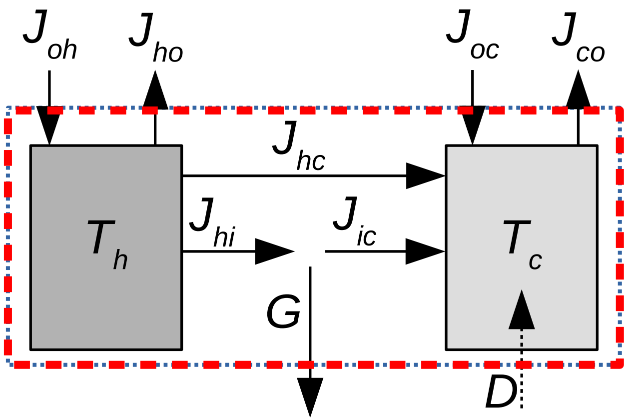
```
class eq_deS(Equation):
    """Entropy exchange of combined system."""
    expr = Eq(deS, (J_oh - J_ho) / T_h + (J_oc + D - J_c
display(eq_deS)

class eq_diS(Equation):
    """Entropy production within combined system"""
    expr = Eq(diS, (J_hc + J_ic) / T_c - (J_hc + J_hi) /
display(eq_diS)
```

Entropy exchange:
Due to fluxes crossing outside boundary (except G)

Entropy production:
Due to fluxes within boundaries

$$d_{eS} = \frac{-J_{ho} + J_{oh}}{T_h} + \frac{D - J_{co} + J_{oc}}{T_c}$$

$$d_{iS} = -\frac{J_{hc} + J_{hi}}{T_h} + \frac{J_{hc} + J_{ic}}{T_c}$$



6. DEFINE ENTROPY PRODUCTION BY EACH FLUX

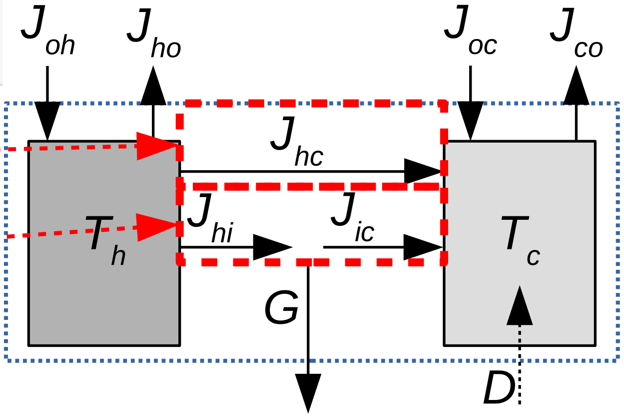
Need to formulate equations for entropy production by each individual flux. Here it is an equation for J_{hc} and another equation for the combination of J_{hi} and J_{ic}.


```
class eq_diS_Jhc(Equation):
    """Entropy production due to J_hc."""
    expr = Eq(diS_Jhc, J_hc/T_c - J_hc/T_h)
display(eq_diS_Jhc)

class eq_diS_Jhi(Equation):
    """Entropy production due to J_hi and J_ic."""
    expr = Eq(diS_Jhi, J_ic/T_c - J_hi/T_h)
display(eq_diS_Jhi)
```

$d_{iS} = d_{iS,Jhc} + d_{iS,Jhi}$

$$d_{iS,Jhc} = -\frac{J_{hc}}{T_h} + \frac{J_{hc}}{T_c}$$

$$d_{iS,Jhi} = -\frac{J_{hi}}{T_h} + \frac{J_{ic}}{T_c}$$



COMPUTE CARNOT-LIMIT OF POWER EXTRACTION FROM HEAT FLUX

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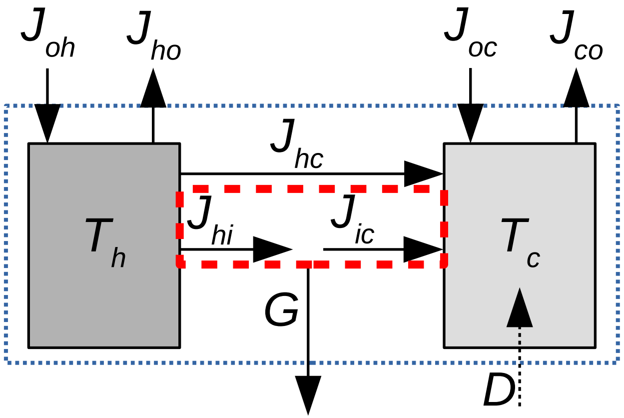
Now calculate the Carnot limit for extracting power from J_{hi}.

Set $d_{iS,Jhi}$ = 0, and solve for G

```
class eq_G(eq_diS_Jhi.definition, eq_Jic.definition):
    """Maximum power (G)."""
    expr = Eq(G, solve([eq_diS_Jhi.rhs, eq_Jic], G, J_ic)[G])
eq_G
```

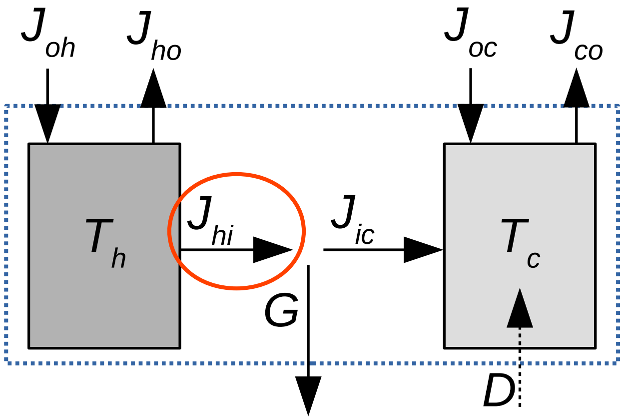
$$G = -\frac{J_{hi} T_c}{T_h} + J_{hi}$$

Carnot limit for extracting power from J_{hi}



POSSIBLE APPLICATION: PREDICT HEAT TRANSFER COEFFICIENT

Similar 2-box model was used by Lorenz et al. (2001, Geophys. Res. Lett., 28(3)), to calculate the equator-pole heat transport of the Earth and other planets. Assume that the atmosphere can optimise the heat transfer coefficient (k_{hi} for J_{hi}).



Assumption:
Heat transfer coefficient a result of self-organised system structure

$$J_{hi} = k_{hi} (T_h - T_c)$$
$$J_{ic} = J_{hi} - G$$

What would be optimal k_{hi} for:

(a) Maximum G at D=0?
(b) Maximum G at D=G?
(c) Maximum diS?

OPTIMAL k_{hi} FOR MP, MP WITH DISSIPATION AND MEP

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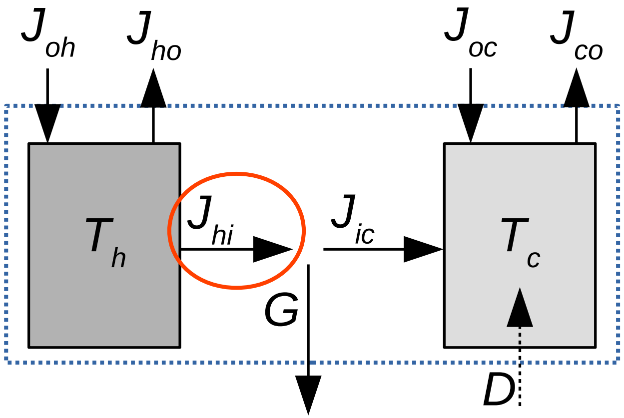
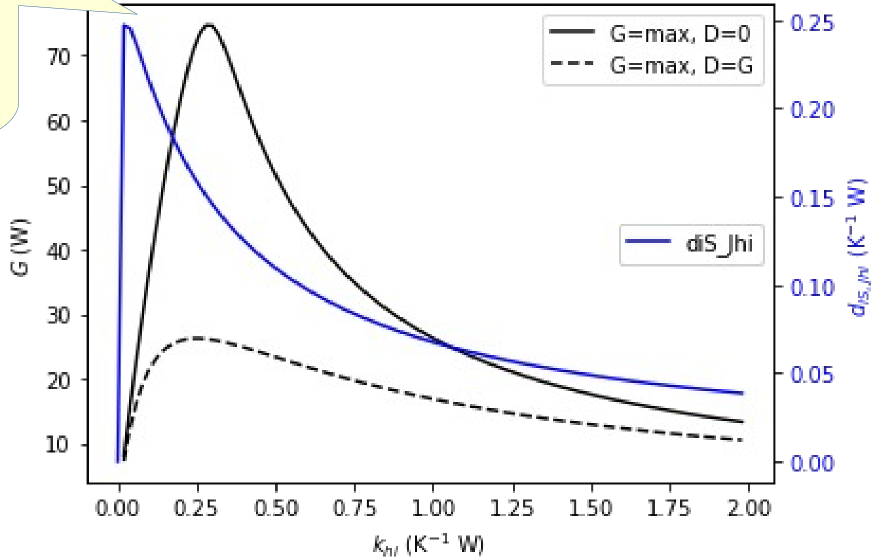
Optimal k_{hi} different for max power with/without dissipation, <u>very different</u> for MEP



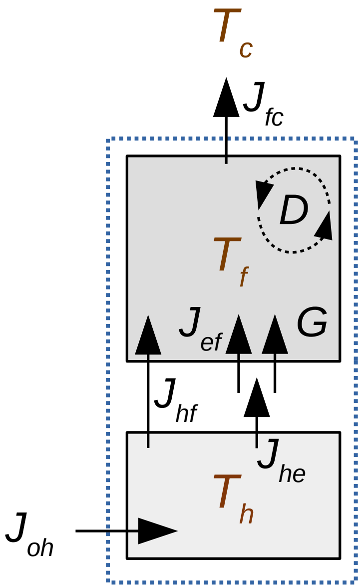


Common B.C.

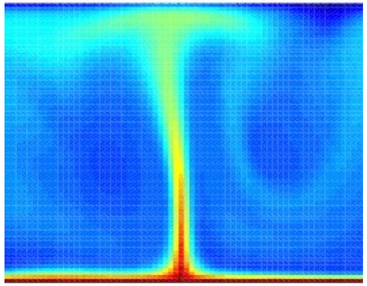
(J_oh, 300.0 W)
(J_oc, 1.0 W)
(k_ho, 0.7 W K^{-1})
(k_hc, 0)
(k_co, 0.3 W K^{-1})

Max. G, D=0	Max. G, D=G	Max. $d_{iS,Jhi}$
(k_hi, 0.29 W K^{-1})	(k_hi, 0.25)	(k_hi, 0.03)
(J_hi, 82.0 W)	(J_hi, 48.6)	(J_hi, 10.0)
(J_ic, 7.2 W)	(J_ic, 22.4)	(J_ic, 10.0)
(G, 74.8 W)	(G, 26.2)	(G, 0)
(T_h, 311.3 K)	(T_h, 359.2)	(T_h, 414.3)
(T_c, 27.5 K)	(T_c, 165.2)	(T_c, 36.5)

OPTIMAL k_{he} IN THERMAL CONVECTION



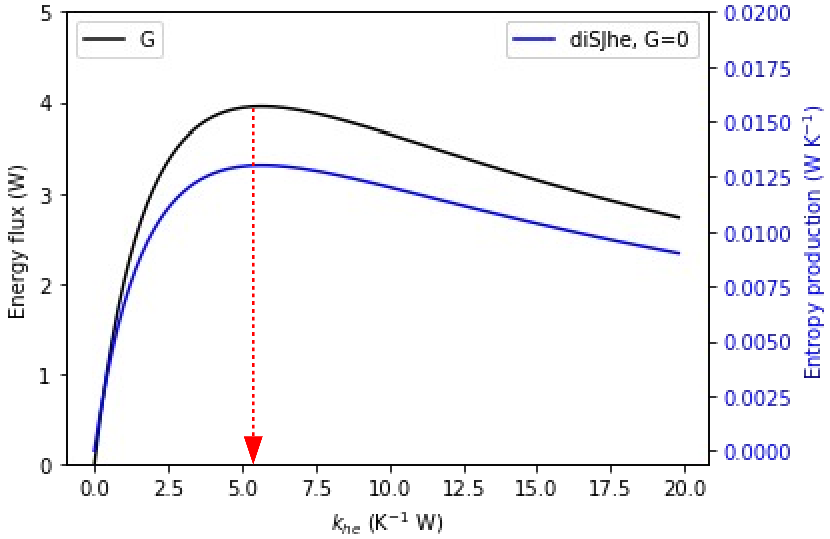
COLD



https://commons.wikimedia.org/wiki/File:Convection-snapshot.png

HOT

→ EXPLANATION



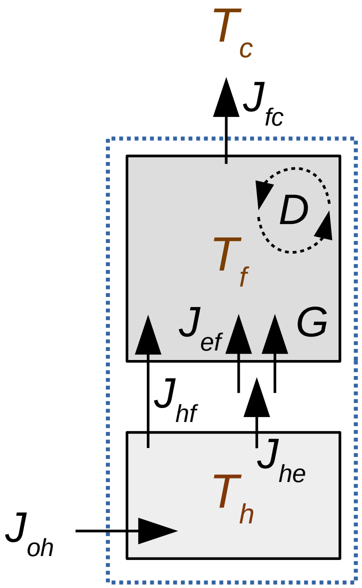
Common B.C.

```
(J_oh, 165.0 W)
(k_hf, 5.4 W K-1)
(T_c, 273.0 K)
(k_fc, 5.4 W K-1)
```

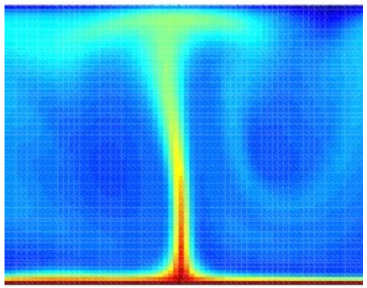
Max. G, D=G	Max. $d_{iS,Jhe}$, G=0
(k_he, 5.67)	(k_he, 5.67)
(G, 3.96)	(G, 0)
(J_he, 84.48)	(J_he, 84.48)
(J_hf, 80.52)	(J_hf, 80.52)
(T_h, 318.47)	(T_h, 318.47)
(T_f, 303.56)	(T_f, 303.56)
(T_c, 273.0)	(T_c, 273.0)

https://renkulab.io/projects/stanislaus.schymanski/thermodynamic_optimality_blueprint/files/blob/notebooks/TD-boxes_convection.ipynb

OPTIMAL k_{he} IN THERMAL CONVECTION

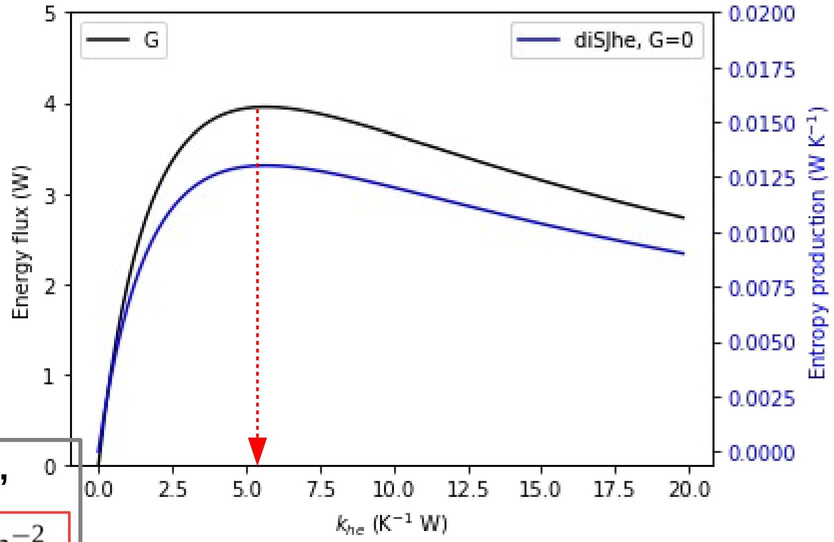


COLD



HOT

https://commons.wikimedia.org/wiki/File:Convection-snapshot.png



→EXPLANATION

Kleidon & Renner, 2017, HESS 17(7)

max. power (dry convection)	$1.5\,\mathrm{W\,m^{-2}}$
max. power (moist convection)	$2.5\,\mathrm{W\,m^{-2}}$
max. power (lifting)	$0.4\,\mathrm{W\,m^{-2}}$
exchange velocity	$1.5\,\mathrm{mm\,s^{-1}}$
terrestrial radiation	$83\,\mathrm{W\,m^{-2}}$
sensible heat	$28\,\mathrm{W\,m^{-2}}$
latent heat	$54\,\mathrm{W\,m^{-2}}$

Common B.C.

```
(J_oh, 165.0 W)
(k_hf, 5.4 W K-1)
(T_c, 273.0 K)
(k_fc, 5.4 W K-1)
```

Max. G, D=G

```
(k_he, 5.67)
(G, 3.96)
(J_he, 84.48)
(J_hf, 80.52)
(T_h, 318.47)
(T_f, 303.56)
(T_c, 273.0)
```

Max. $d_{iS,Jhe}$, G=0

```
(k_he, 5.67)
(G, 0)
(J_he, 84.48)
(J_hf, 80.52)
(T_h, 318.47)
(T_f, 303.56)
(T_c, 273.0)
```

SUMMARY & CONCLUSIONS

LUXEMBOURG INSTITUTE OF SCIENCE AND TECHNOLOGY
LIST
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- Blueprint for thermodynamically self-consistent box models
  - Define internal and external system boundaries
  - Energy balance
  - Entropy balance
  - Entropy production for each individual flux
  - Analytical solutions for steady-state

Use me, I'm interactive!

- Power has to be dissipated **outside** of engine

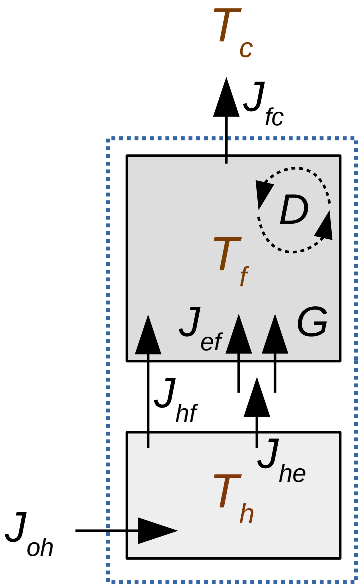
- **MP and MEP can give very different results**

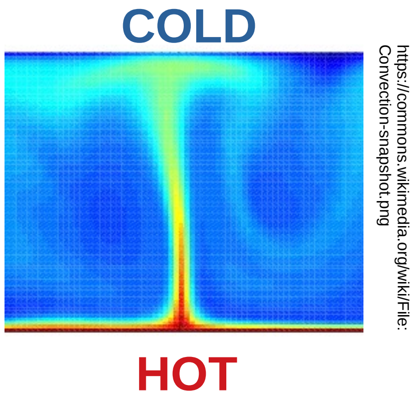
TD-optimality principles are falsifiable hypotheses!

APPENDIX...

The following slides contain some additional explanations and are linked to directly from the related slide in the main presentation. Click on the "BACK" button to return to the original slide.

OPTIMAL k_{he} IN THERMAL CONVECTION





← BACK to slide

Consider thermal convection from a hot surface through a fluid with temperature T_f to a cold surface at the top. Here, we generate convective power right at the surface and the power is injected into the fluid (leading to eddies), where it is also dissipated, here expressed as *D* inside the fluid box. We also have a radiative heat loss both from the surface and at the top of the fluid. We can see that in this case, the optimal heat transfer coefficient maximising either G or entropy production is the same.

Common B.C.

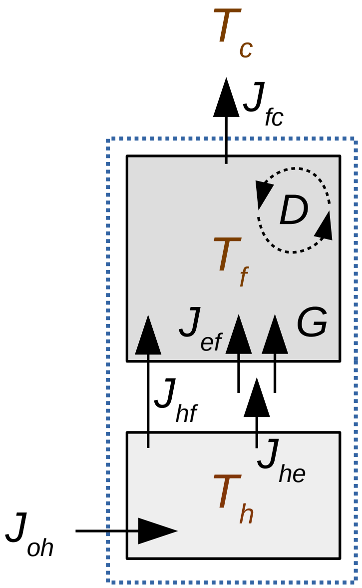
```
(J_oh, 165.0 W)
(k_hf, 5.4 W K⁻¹)
(T_c, 273.0 K)
(k_fc, 5.4 W K⁻¹)
```

Max. G, D=G	Max. $d_{iS,Jhe}$, G=0
(k_he, 5.67)	(k_he, 5.67)
(G, 3.96)	(G, 0)
(J_he, 84.48)	(J_he, 84.48)
(J_hf, 80.52)	(J_hf, 80.52)
(T_h, 318.47)	(T_h, 318.47)
(T_f, 303.56)	(T_f, 303.56)
(T_c, 273.0)	(T_c, 273.0)

https://renkulab.io/projects/stanislaus.schymanski/thermodynamic_optimality_blueprint/files/blob/notebooks/TD-boxes_convection.ipynb

OPTIMAL k_{he} IN THERMAL CONVECTION

- Motivation
- MP vs. MEP
- Drawings
- Blueprint
- **Examples**
- Conclusions

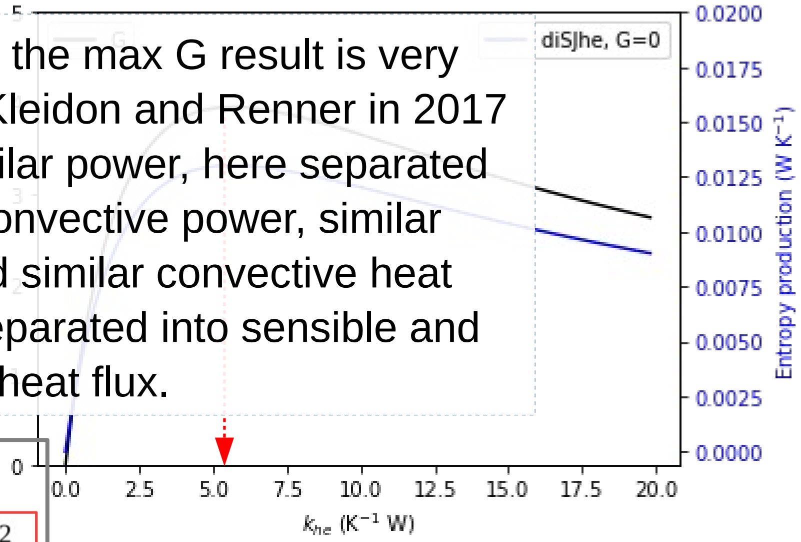


← BACK to slide

Common B.C.

```
(J_oh, 165.0 W)
(k_hf, 5.4 W K⁻¹)
(T_c, 273.0 K)
(k_fc, 5.4 W K⁻¹)
```

We can also see that the max G result is very similar to the result by Kleidon and Renner in 2017 who obtained very similar power, here separated into dry and moist convective power, similar radiative transfer and similar convective heat transfer, here again separated into sensible and latent heat flux.



Kleidon & Renner, 2017, HESS 17(7)

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Max. $d_{iS,Jhe}$, G=0

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