Non-Equilibrium Thermodynamics for Engineers

”How do we find the optimal process unit?”

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Why is the entropy production important?

- The work output from the maximum available

$$w = w_{\max} - w_{lost}$$

- Guy-Stodola’s theorem (1889, 1910):

$$w_{lost} = T_0 (dS_{irr} / dt) > 0 \qquad dS_{irr} / dt = \int \sigma \, dV$$

Mathematical methods for constrained optimisation

Euler Lagrange optimisation:

$$L = \frac{dS_{irr}}{dt} + \sum_i \lambda_i P_i$$

Constraint examples:

$$P = P_1$$

$$T_a = T_0$$

- Conservation equations are included in the objective function

Control theory

$$H = \sigma(z,t) + \sum_i \lambda_i (z,t) f_i$$

Energy balance $f_T = \frac{dT}{dz} = ...$

Momentum balance $f_p = \frac{dp}{dz} = ...$

Mass balance $f_\xi = \frac{d\xi}{dz} = ...$

Extra conditions, i.e. $p_{ext} = const.$

- Local control of conservation equations
- Defined control variables give a practical handle
- Mathematically robust
- An autonomous Hamiltonian is constant along the path

Cf. Course on ”Engeering Fundamentals”
Lectured by prof. J. Gross

Optimal isothermal expansion (1)

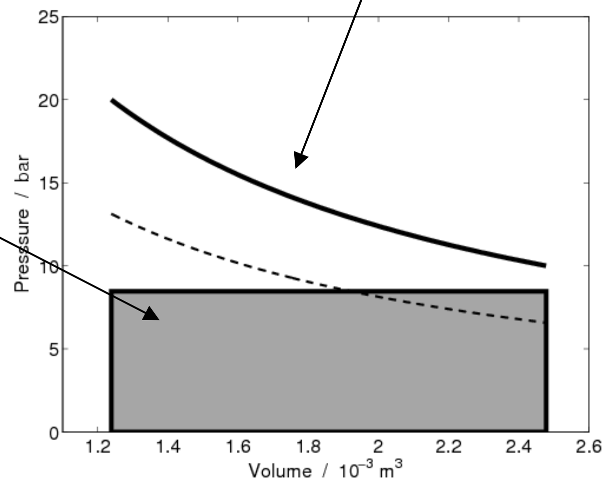
- Find the external pressure in a one step process that gives mininmum lost work, when the pressure of the system changes from V_1 to V_2

N moles of ideal gas in a piston

$$w_{\max} = NRT_0 \ln \frac{p_2}{p_1}$$

$$w = -\int_{V_1}^{V_2} p_{ext} dV = -NRT_0 (\frac{1}{p_2} - \frac{1}{p_1})$$

$$w_{lost} = w - w_{\max} = -NRT_0 \left[p_{ext} (\frac{1}{p_2} - \frac{1}{p_1}) + \ln \frac{p_2}{p_1} \right]$$



The piston moves with time:

$$\frac{dV(t)}{dt} = -\frac{f}{\left[p(t)\right]^2} \left(p_{ext}(t) - p(t) \right)$$

Optimal isothermal expansion (2)

- Which p_{ext} gives minimum entropy production, given the values of p_1 and p_2?

N moles of ideal gas in a piston

$$w_{\max} = NRT_0 \ln \frac{p_2}{p_1}$$

Min

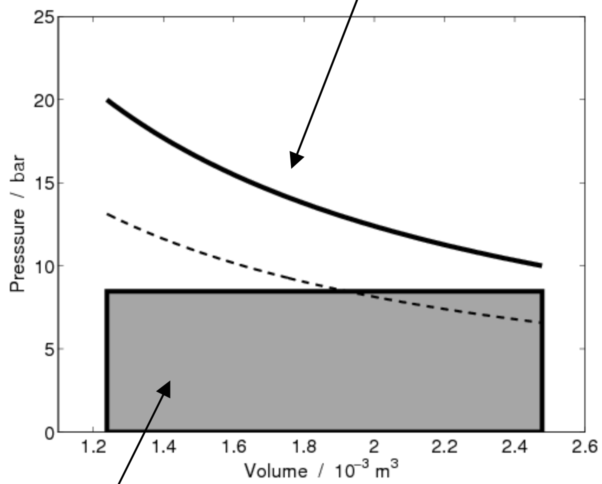
$$\left(\frac{dS_{irr}}{dt} = -NR \left[p_{ext} \left(\frac{1}{p_2} - \frac{1}{p_1} \right) + \ln \frac{p_2}{p_1} \right] \right)$$

Given p_1, p_2

Solution:

$$p_{ext} \quad p_1 \quad \frac{(p_2 / p_1)}{\quad}$$

$$\exp\left(\frac{f}{NRT_0} \right)$$



$$w = -\int_{V_1}^{V_2} p_{ext} dV = -NRT_0 \left(\frac{1}{p_2} - \frac{1}{p_1} \right)$$

Optimal isothermal expansion (3)

The pressure variation giving minimum lost work (stipled line) can be obtained from control theory

General objective function:

$$\frac{dS_{irr}}{dt} = \int_0^{\theta} \frac{1}{T_0}\left(p_{ext}(t) - p(t)\right)\left[-\frac{dV(t)}{dt}\right]$$

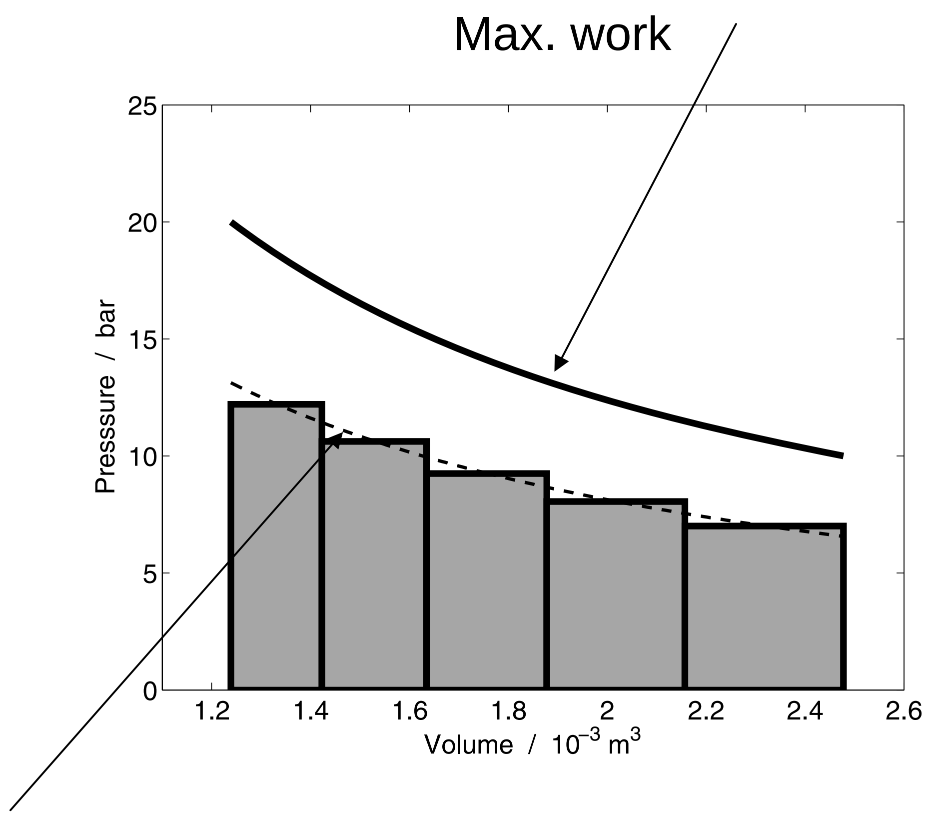
Constraint:

$$\frac{dV(t)}{dt} = -\frac{f}{\left[p(t)\right]^2}\left(p_{ext}(t) - p(t)\right)$$

Solution:

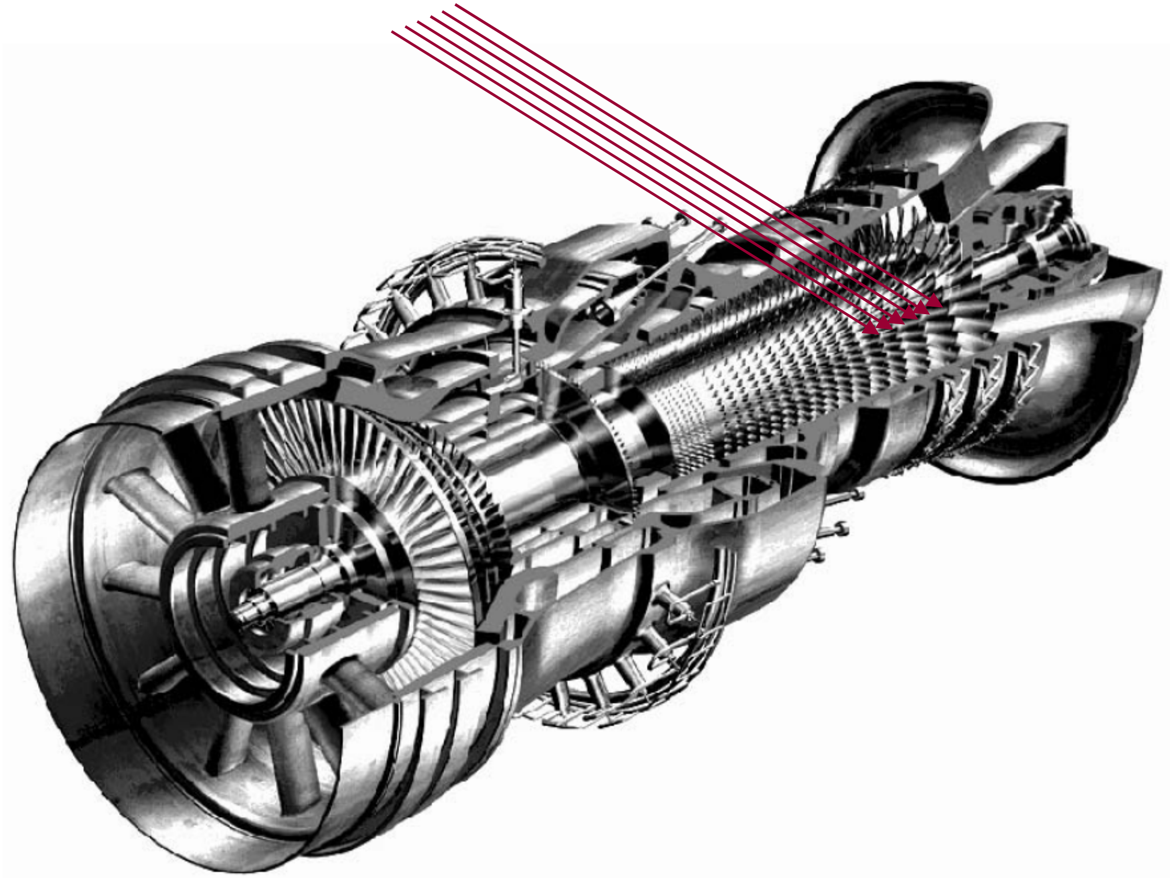
$$p_{ext} = p_1\left(1 + \frac{NRT_0}{f\theta}\ln\frac{p_2}{p_1}\right)\left(\frac{p_2}{p_1}\right)^{t/\theta}$$

$$p(t) = p_1\left(\frac{p_2}{p_1}\right)^{t/\theta}$$



The driving force is constant along the optimal path, and so is σ!

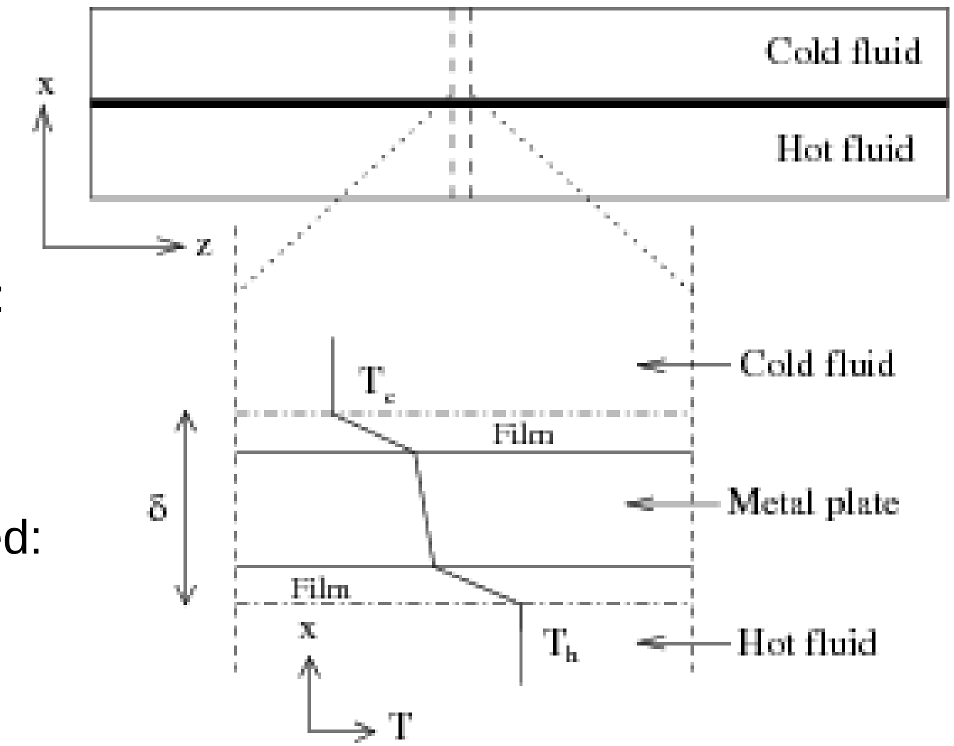
Optimal expansion (4):
Continuous Expansion of Gases in a Turbine



„Multistage“ gas turbine – a realization of the results derived for the K-step expansion case?

Optimal heat exchange (1)

- **Find the temperature profile *T(z)* that gives minimum entropy production, when a given amount of heat is transferred from the hot fluid**



Constraints

Fixed heat transferred means fixed:

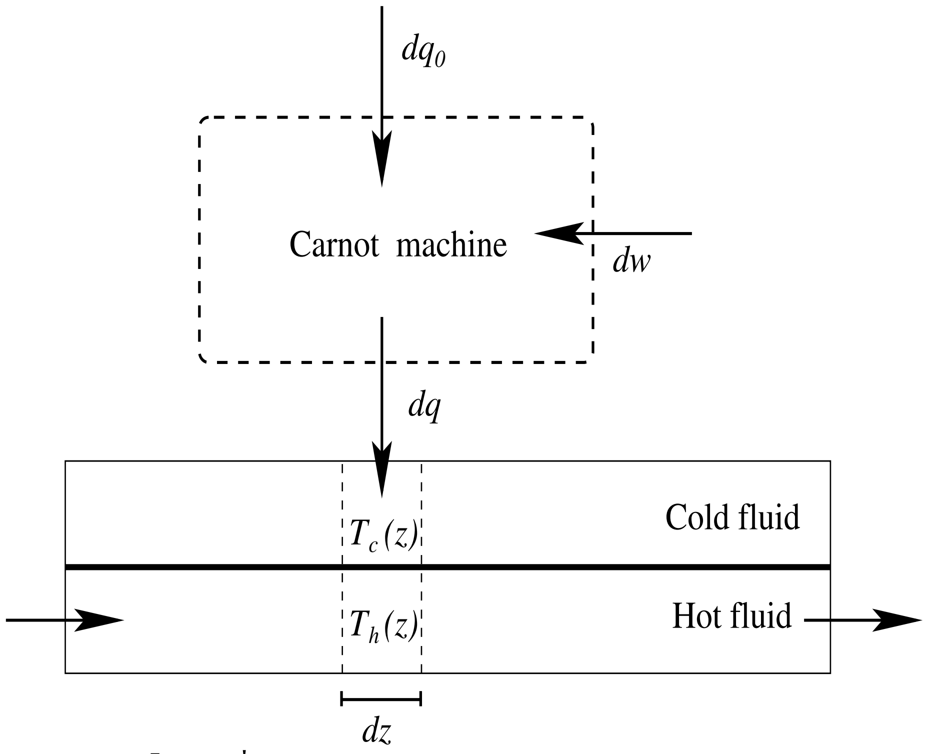
$$T_{h,in} \text{ and } T_{h,out}$$

The energy balance must be obeyed:

$$FC_p dT_h(z) = J_q^{'}(z)\Delta y dz$$

Optimal heat exchange (3):
Is work is obtainable by heat exchange?

$$\frac{dq_0}{T_0} = \frac{dq}{T_c(z)} \qquad dq = J_q^{'}(z)\Delta y dz$$



$$dw = \eta_C dq = \Delta y \left[1 - \frac{T_0}{T_c(z)} \right] J_q^{'} dz$$

$$w = \Delta y \int_0^L \left[1 - \frac{T_0}{T_c(z)} \right] J_q^{'} dz = F_{out} H_{out} - F_{in} H_{in} - \Delta y T_0 \int_0^L \frac{J_q^{'}}{T_c(z)} dz$$

Entropy production from transfer to cold side

Optimal heat exchange (2): The entropy production

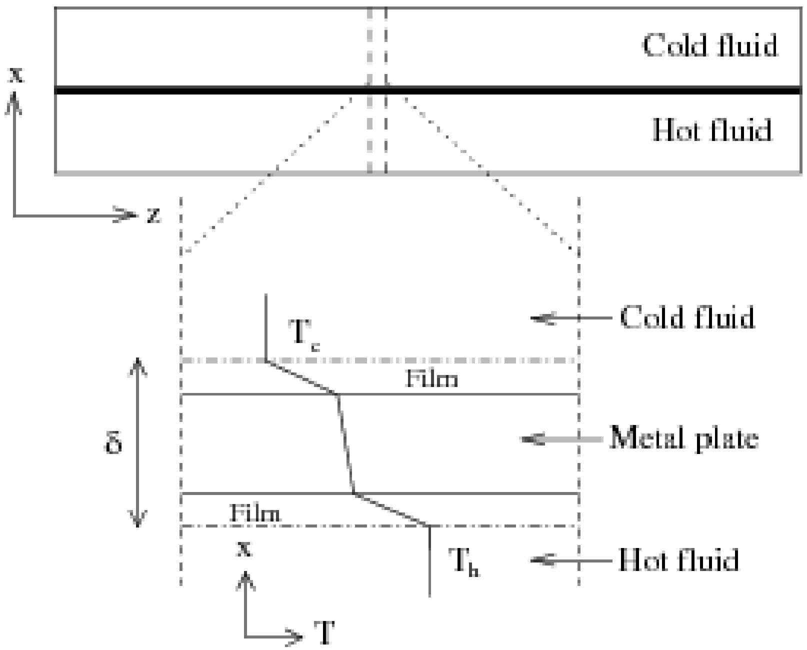
$$(x,z) \quad J_q^{'}(x,z)\frac{d}{dx} \quad \frac{1}{T(x,z)}$$

$$J_q^{'}(x,z) \quad J_q^{'}(z)$$

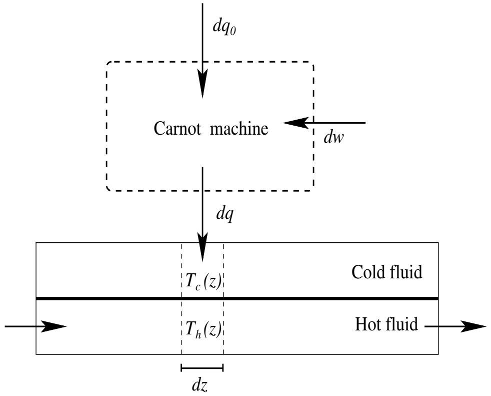
$$(z) \quad y_{\;0} \quad (x,z)dx \quad yJ_q^{'}(z) \quad \frac{1}{T_h(z)} \quad \frac{1}{T_c(z)}$$

$$J_q^{'} = l_{qq}\Delta\left(\frac{1}{T}\right)$$

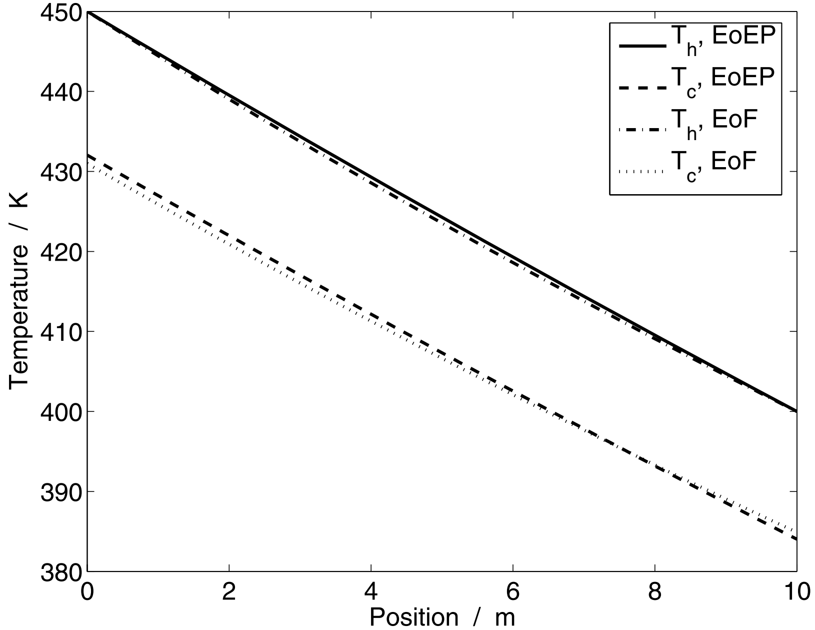
$$\frac{dS_{irr}}{dt} = \Delta y\int_0^L \sigma(z)dz = \Delta y\int_0^L \left(l_{qq}\right)^{-1}\left[J_q^{'}\right]^2 dz$$



Optimal heat exchange (5): Solution



- Exact solution: Constant entropy production (EoEP)
- Approximate solution: Constant thermal force (EoF)



The entropy balance for the hot fluid

$$\frac{dS_{irr}}{dt} = F_{out}S_{out} - F_{in}S_{in} - \Delta y \int_0^L \frac{J_q^{'}}{T_c(z)} dz$$

The entropy production for heat exchange

$$\frac{dS_{irr}}{dt} = \Delta y \int_0^{\delta} \int_0^L \sigma(x,z) dz dx = \Delta y \int_0^L \sigma(z) dz$$

$$= \Delta y \int_0^L l_{qq}(T_h(z)) \left[\Delta \frac{1}{T} \right]^2 dz$$

Reasons to minimize the entropy production

- We obtain a realistic target for the efficiency:
  The most energy efficient operation for the real system
- We find a zero on a yardstick that measures lost work
- We can find rules for process design:

Rules of thumb, energy efficient design

- A turbine with equipartition of forces
- Heat exchange with equipartition of forces

Energy efficient design means that:

1. The path of minimum entropy production has been used, given the boundary conditions
2. This operating path has constant entropy production if the system has sufficient degrees of freedom
3. Constant driving forces seems to be a good approximation to a state with constant entropy production