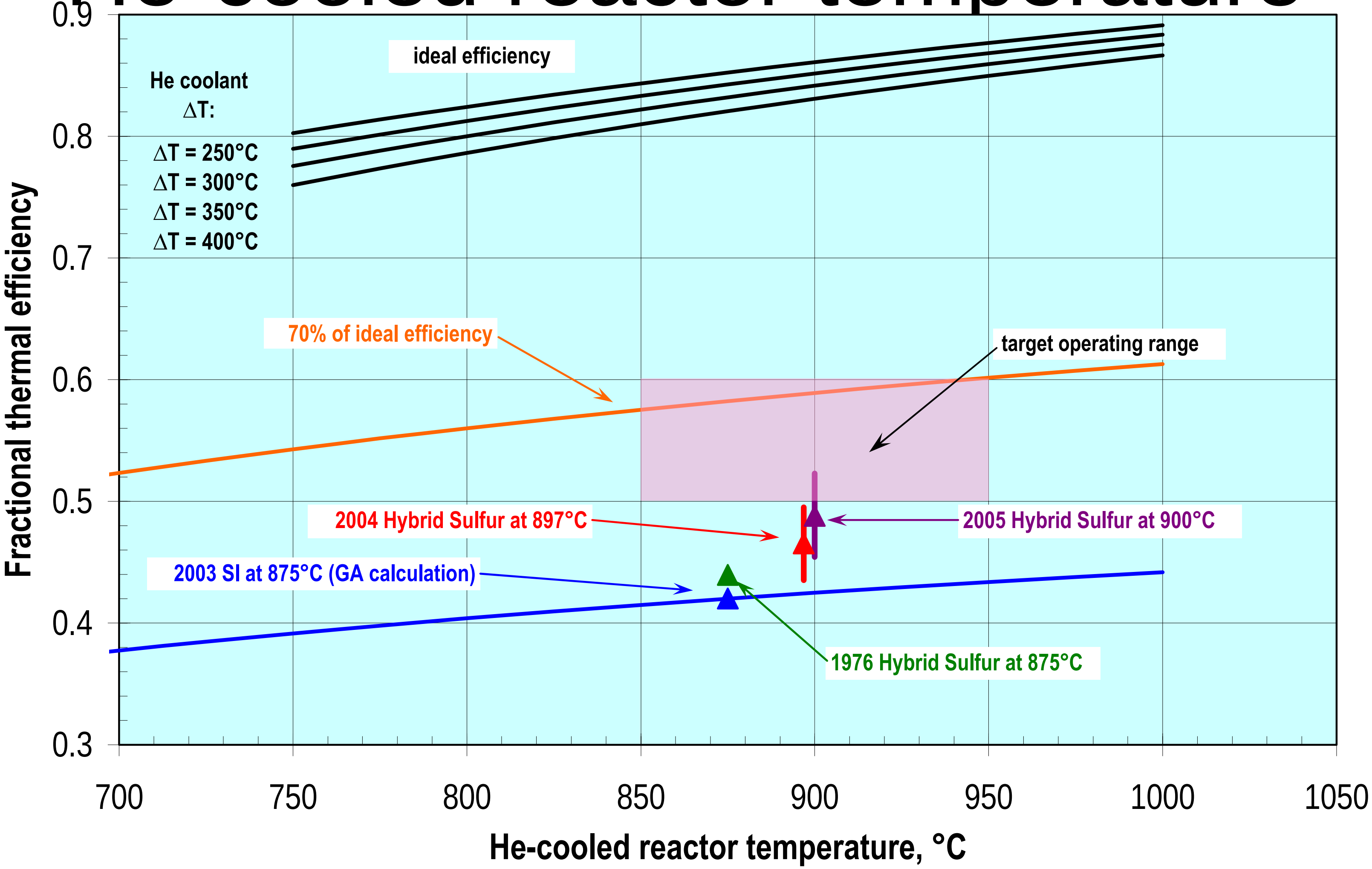
Thermodynamic Efficiency Analysis of the S-I Process for Nuclear Hydrogen Production

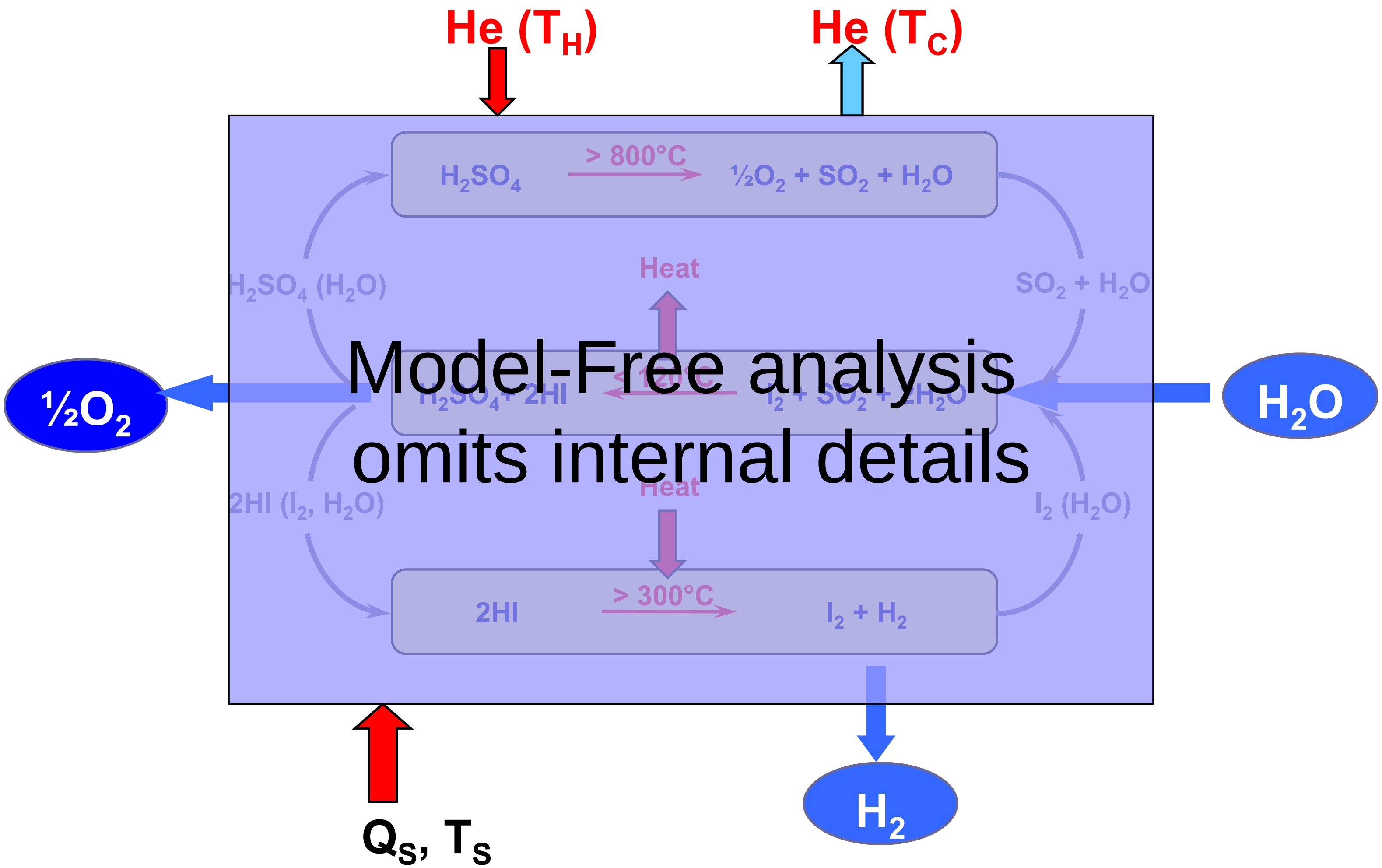
J.P. O'Connell, **K.P. Bellezza**, **P. Narkpresert**, U. Virginia
M.B. Gorensek, Savannah River National Laboratory
P.M. Mathias, Independent Consultant

Work performed under DE-FC07-51D14677

Thermal efficiency as a function of He-cooled reactor temperature



Sulfur-Iodine (SI) Thermochemical Cycle for H_2 Production



OBJECTIVES

- Set up procedure for, & obtain, reversible process limits for idealized & simulated Sulfur-Iodine H_2 generation sections
- Minimize influence of model properties & process units – “model-free”
- Use as basis to compare effects on efficiency of configurations & flows
- Determine sensitivities to guide data taking for reliable simulations
- Perhaps suggest novel process concepts

GENERAL APPROACH

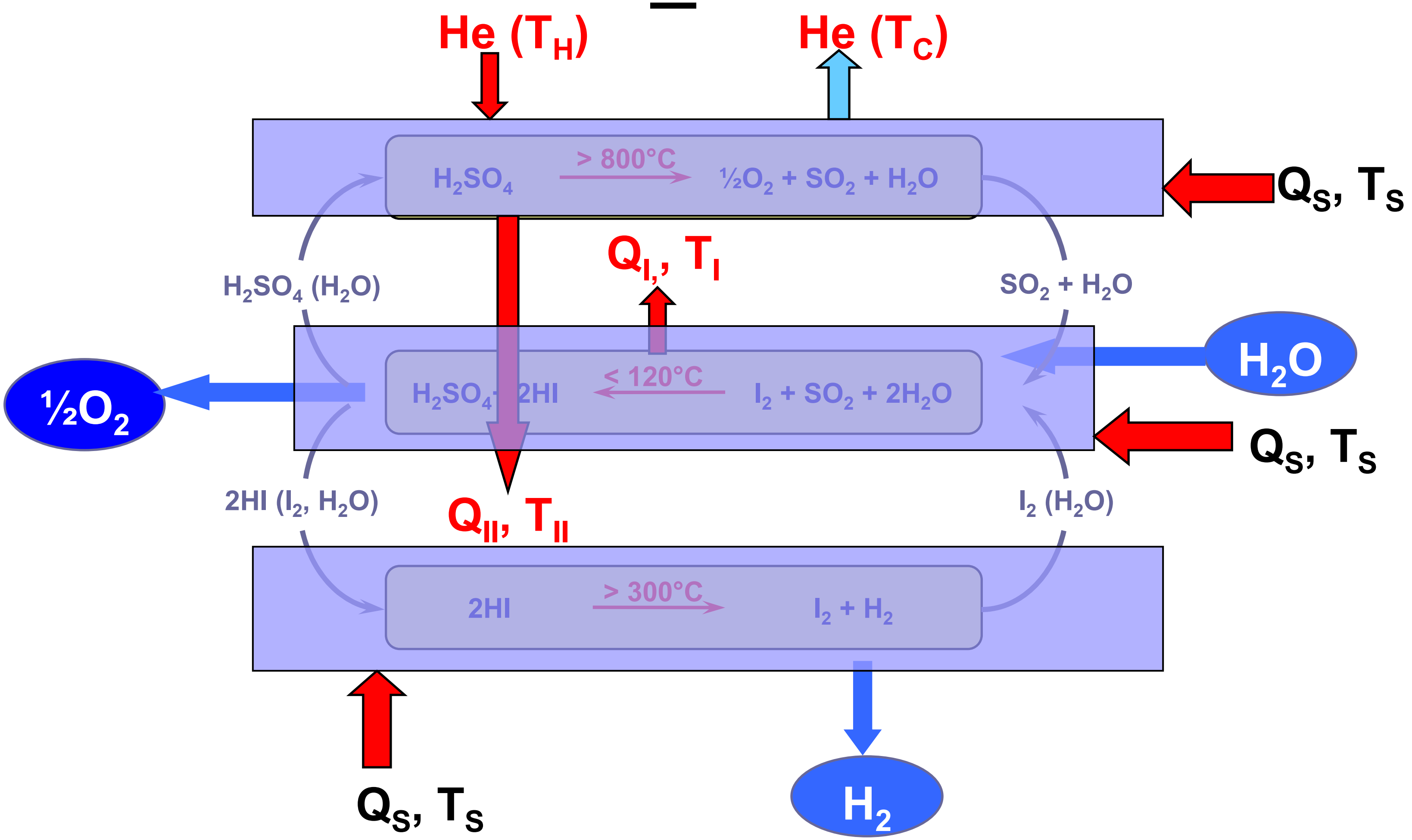
- Use steady-state 1st & 2nd Law equations for reversible/reversible systems with material & energy flows on sections & overall process
- 1st Law

$$\sum_{inlet\ ports} \dot{n}h_i - \sum_{outlet\ ports} \dot{n}h_o + \sum_{heats} \dot{Q}_H + \sum_{machines} \dot{W} = 0$$

- 2nd Law (reversible for $\dot{S}_{gen} = 0$)

$$\sum_{inlet\ ports} \dot{n}s_i - \sum_{outlet\ ports} \dot{n}s_o + \sum_{heats} \frac{\dot{Q}_H}{T_H} + \dot{S}_{gen} = 0$$

Sulfur-Iodine (SI) Thermochemical Cycle for H_2 Production

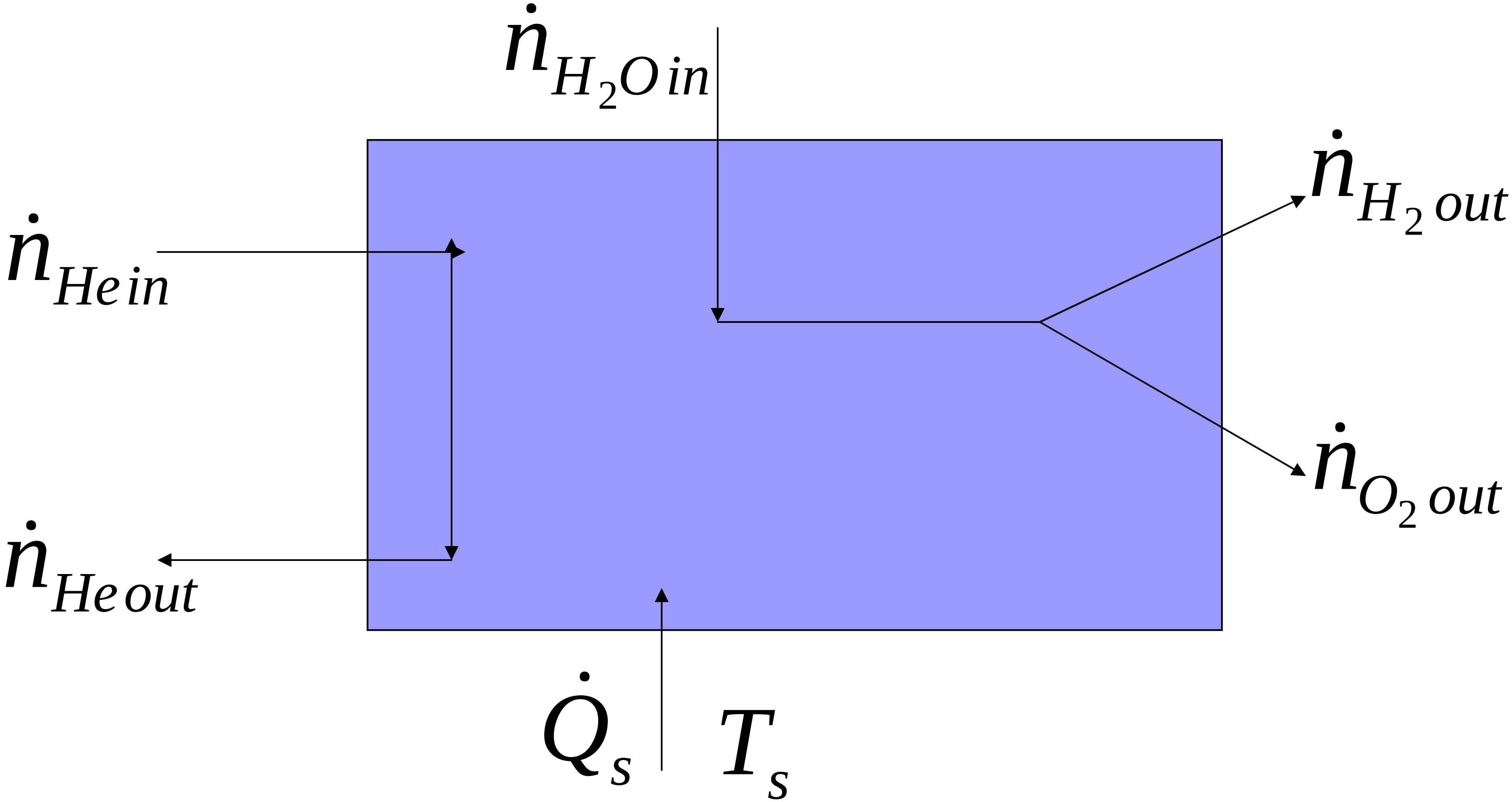


Use Analysis to Determine Q_i, Q_S of Sections

SOLVE FOR 2 VARIABLES

- Variables:
  - Inlet/outlet streams: *T*, *P*, $\dot{n}_i, \dot{n}_o$
  - Heat effects: $\dot{Q}_I$ & $\dot{Q}_S$
- Use property model relations for reaction & stream enthalpies, *h*, entropies, *s*
- Use 2 equations to solve for 2 variables of:
  - Overall water-splitting system
  - S-I sections I-III with only reactant/products
  - S-I sections I-III with recycled components
- For reversible compared to real, 1 condition different
- For irreversible what S_{gen} matches real conditions?

OVERALL WATER SPLITTING



$$\dot{n}_{He\,out} = \dot{n}_{He\,in} \qquad \dot{n}_{H_2\,out} = 2\dot{n}_{O_2\,out} = \dot{n}_{H_2O\,in} = 1\ \text{kmol/hr}$$

WATER SPLITTING BALANCES

$$\dot{n}_{He\ in}(h_{He\ in} - h_{He\ out}) - \dot{n}_{H_2\ out}(h_{H_2\ out} + \frac{1}{2}h_{O_2\ out} - h_{H_2O\ in}) + \dot{Q}_s = 0$$

$$\dot{n}_{He\ in}c_{p,He}(T_{He\ in} - T_{He\ out}) - \dot{n}_{H_2\ out}\Delta H_{WS} + \dot{Q}_s = 0$$

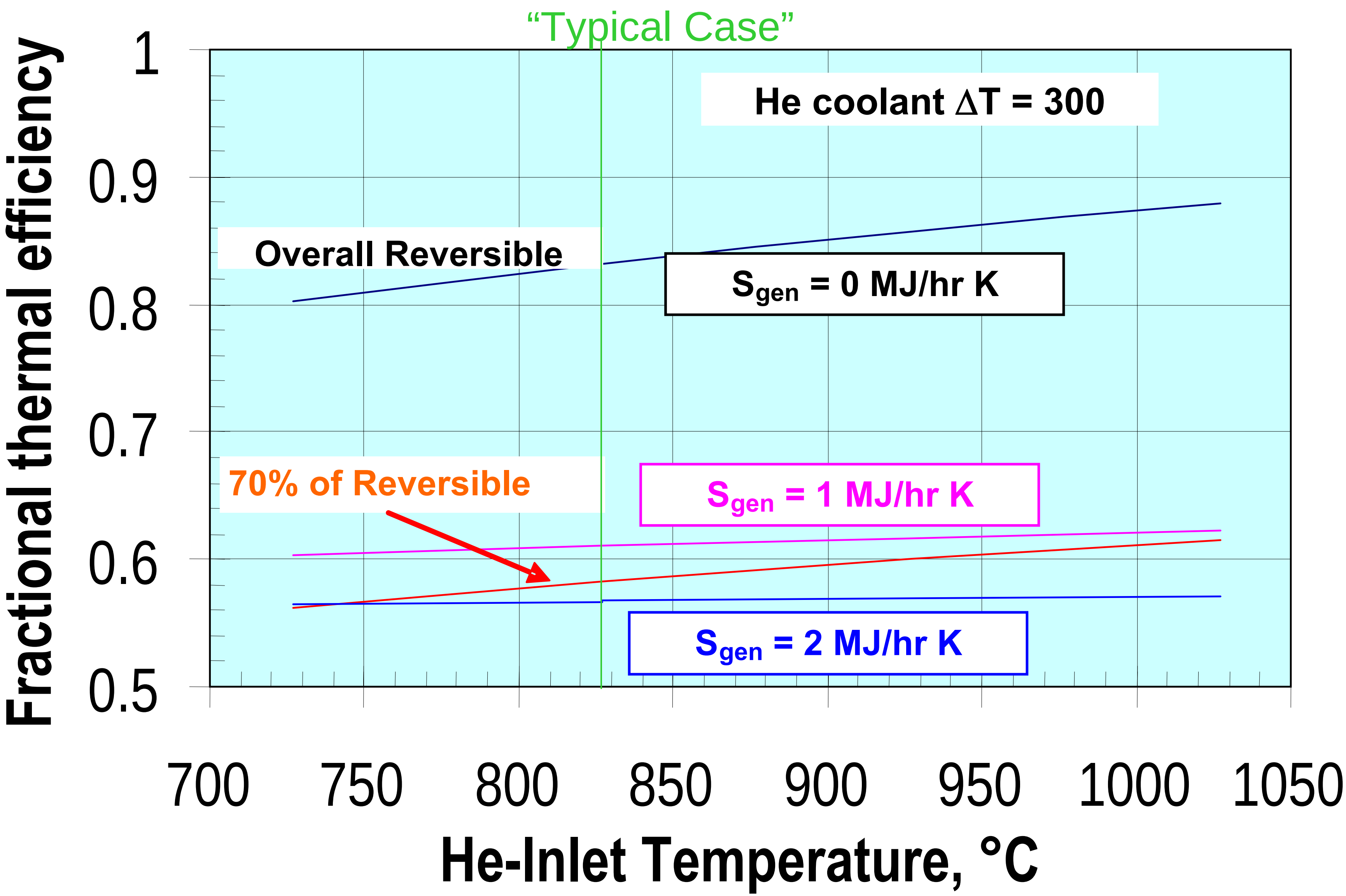
$$\dot{n}_{He\ in}(s_{He\ in} - s_{He\ out}) - \dot{n}_{H_2\ out}(s_{H_2\ out} + \frac{1}{2}s_{O_2\ out} - s_{H_2O\ in}) + \frac{\dot{Q}_s}{T_s} + S_{gen} = 0$$

$$\dot{n}_{He\ in}\left[c_{p,He}\ln\left(\frac{T_{He\ in}}{T_{He\ out}}\right) - R\ln\left(\frac{P_{He\ in}}{P_{He\ out}}\right)\right] - \dot{n}_{H_2\ out}\Delta S_{WS} + \frac{\dot{Q}_s}{T_s} + S_{gen} = 0$$

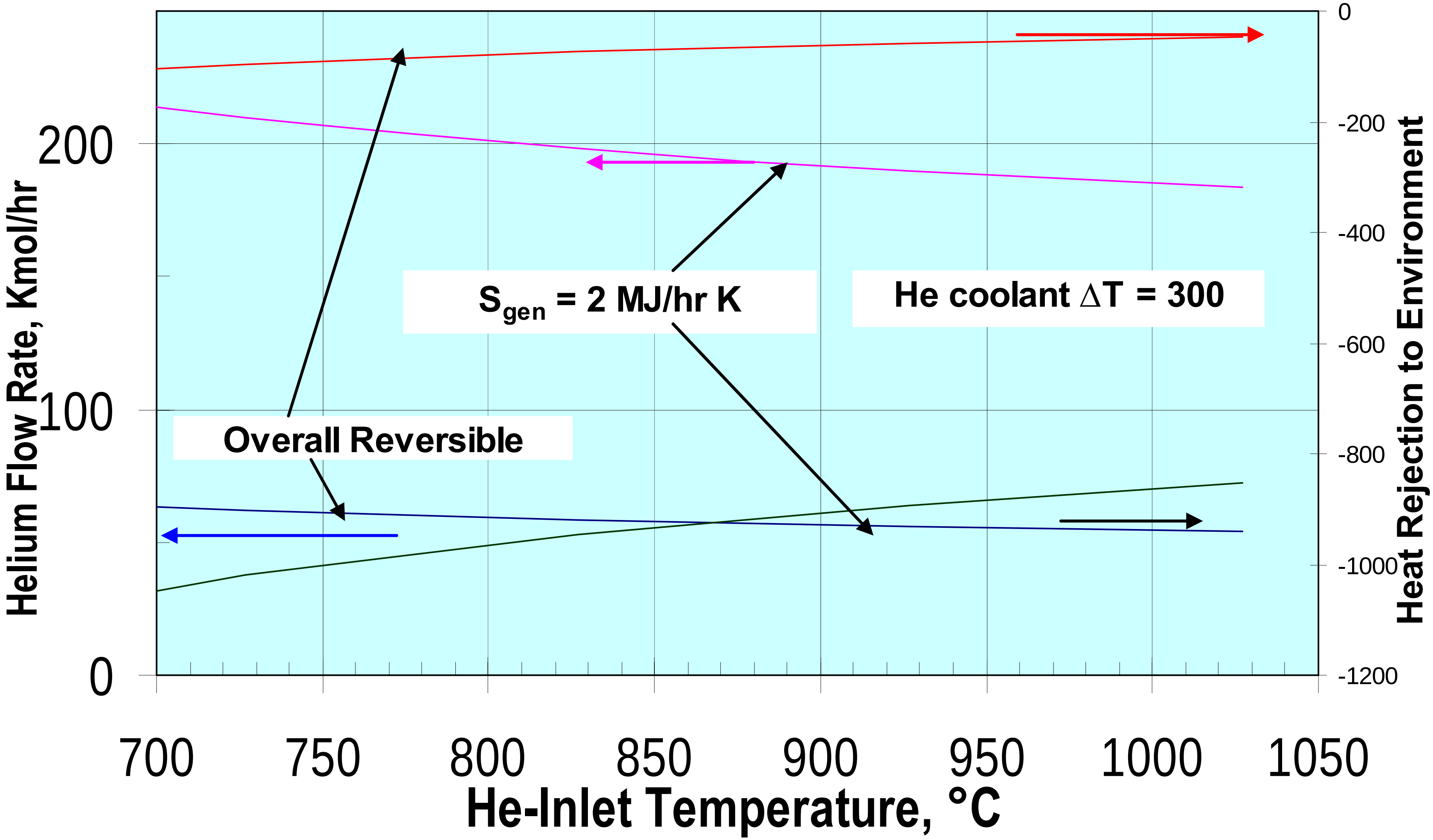
Choose $T_{He\ out}$, $P_{He\ out}$, $P_{He\ in}$, T_s; range of $T_{He\ in}$

Set $c_{p,\ He}$, ΔH_{WS}, ΔS_{WS}, S_{gen} Solve for $\dot{Q}_s$ & $\dot{n}_{He\ in} \Rightarrow \eta$

OVERALL WATER SPLITTING



He & Heat Flows for Water-Splitting



EQUATIONS FOR SECTIONS

Reversible

- 1st Law

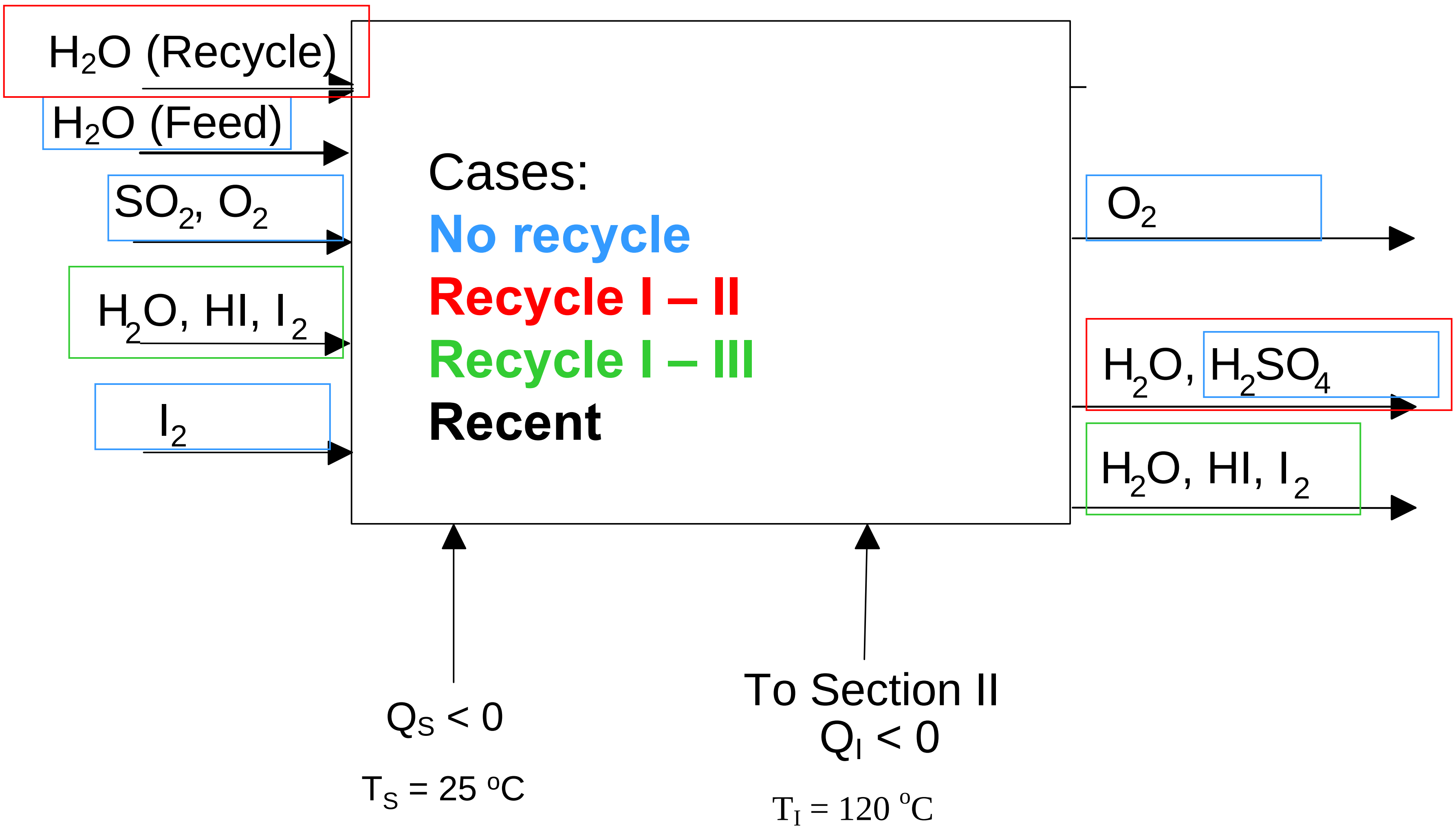
$$\sum_{\text{inlet ports}} \dot{n}h_i - \sum_{\text{outlet ports}} \dot{n}h_o + \dot{Q}_I + \dot{Q}_S = 0$$

Irreversible

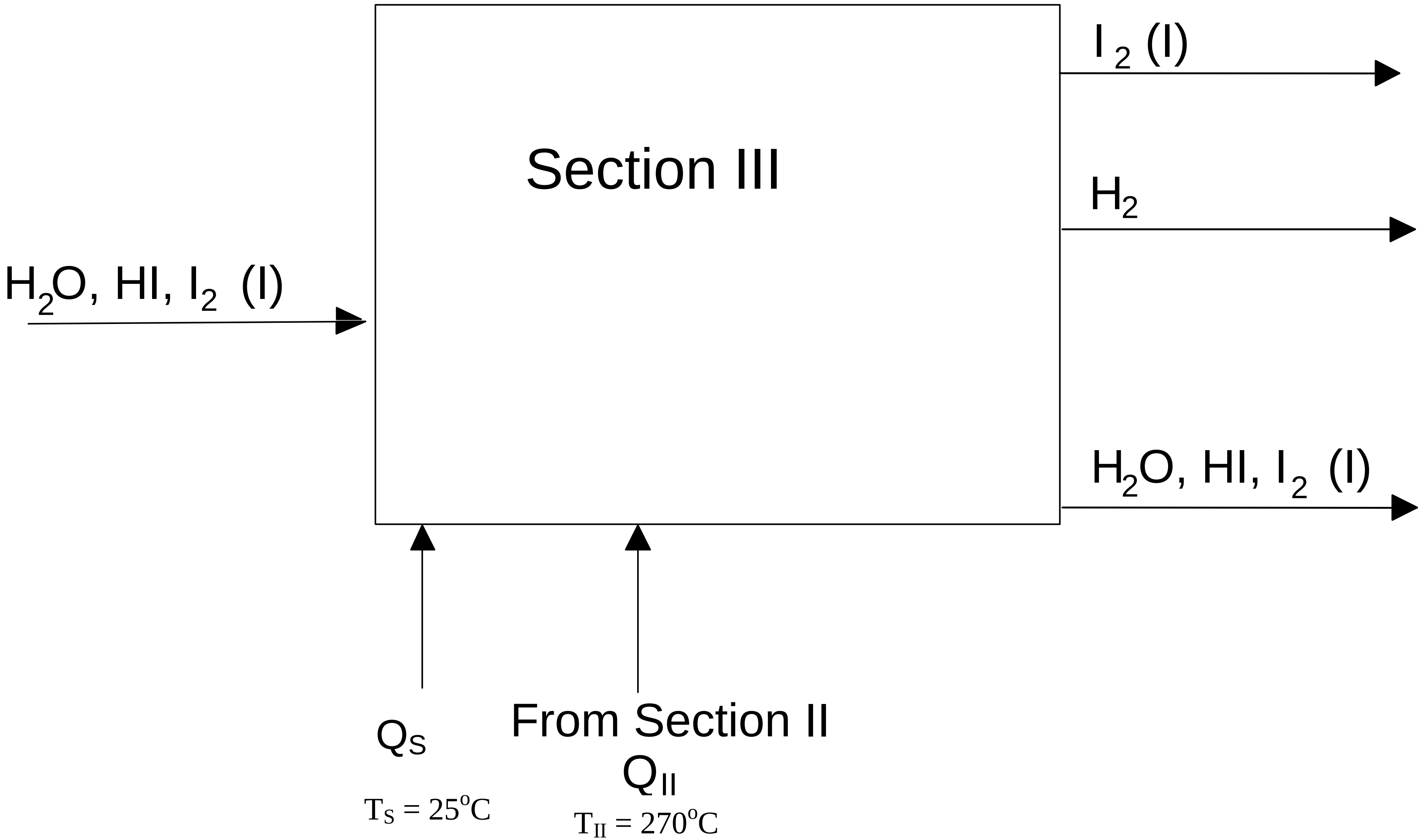
- 2nd Law (reversible for $\dot{S}_{gen} = 0$)

$$\sum_{\text{inlet ports}} \dot{n}s_i - \sum_{\text{outlet ports}} \dot{n}s_o + \frac{\dot{Q}_I}{T_I} + \frac{\dot{Q}_S}{T_S} + \dot{S}_{gen} = 0$$

MATERIAL FLOWS SECTION I



MATERIAL FLOWS SECTION III



TYPICAL SECTION RESULTS

Case	Q_I to II MJ/hr	Q_{II} to III MJ/hr	Q_S MJ/hr	He Flow Kmol/hr
Reversible (S_{gen} = 0) $T_{He\ In} = 827^oC$; $T_{He\ Out} = 527^oC$				

CONCLUSIONS

- Model-free analysis shows
  - Overall process can have high efficiency
  - For reversible sections, adding recycles leads to large internal heat flows,
    unchanged He flow & heat rejection
  - For irreversible sections, internal heat flows further increased, He flow & heat rejection much greater
    - Section I-II recycle has less effect than I-III
- Further study to uncover sensitivities, specific locations for efficiency focus