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

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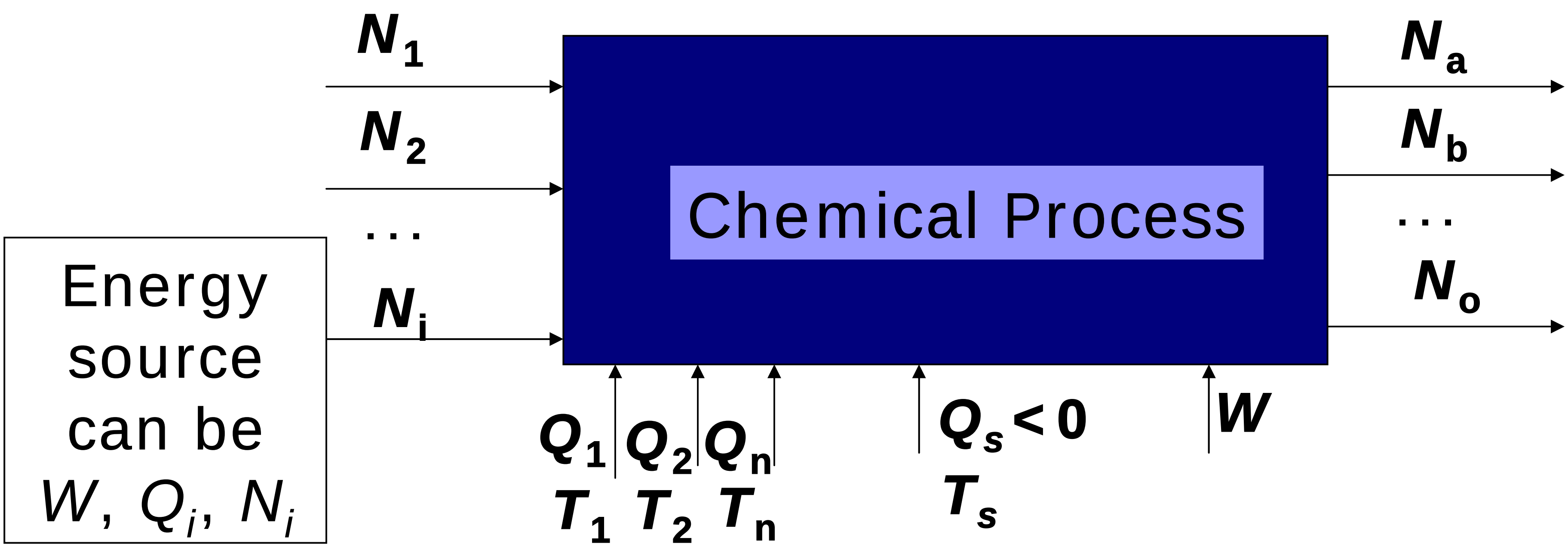
RESEARCH OBJECTIVES

- Develop generalized methodology for analyzing efficiencies resulting from:
  - Alternative process options for material stream rates & conditions, heat & work flows
  - Different property models
- Minimize influence of process model equipment & configuration – “model-free”
- Standardize basis for comparing efficiencies
- Determine sensitivities to guide experiment & process simulations

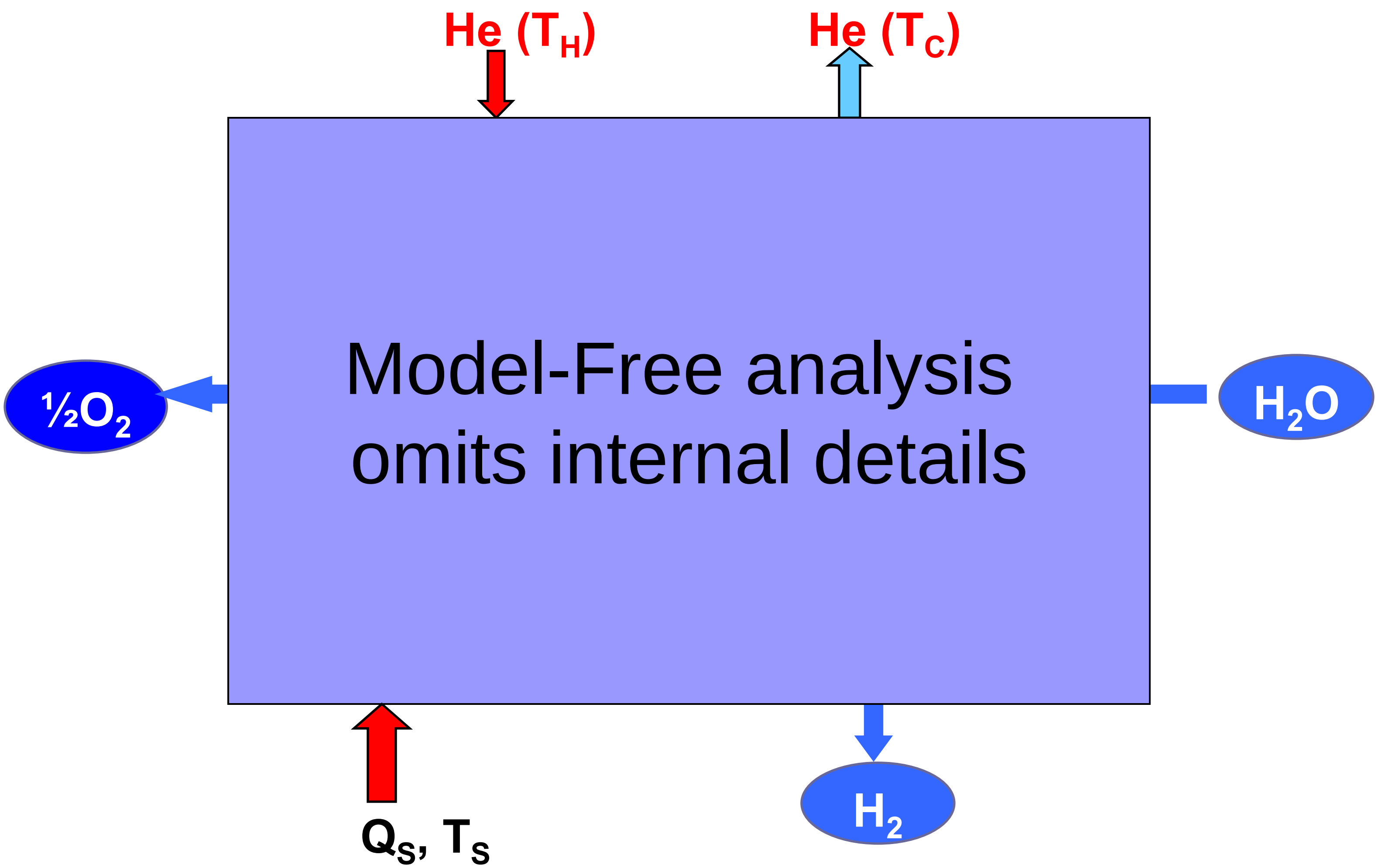
OBJECTIVES OF TALK

- Extend previous work on reversible limits for idealized & simulated General Atomics S-I process for H_2 generation
- Evaluate ideal & real alternative processes – GA & JAERI
- Examine results from different property models - Aspen & OLI

PROCESS MODEL-FREE ANALYSIS



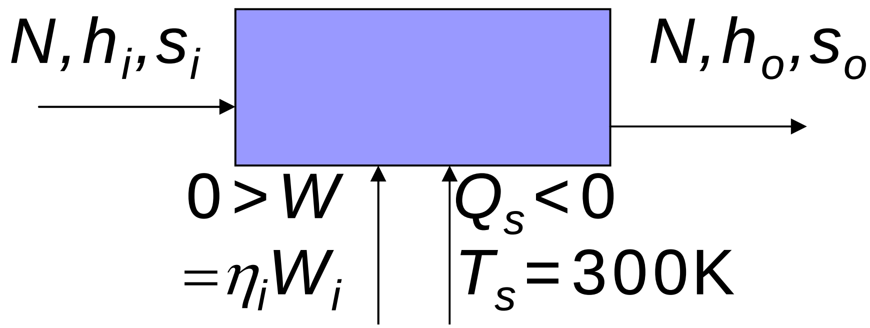
Sulfur-Iodine (SI) Thermochemical Cycle for H_2 Production



TO GET A FEELING FOR S_{GEN}

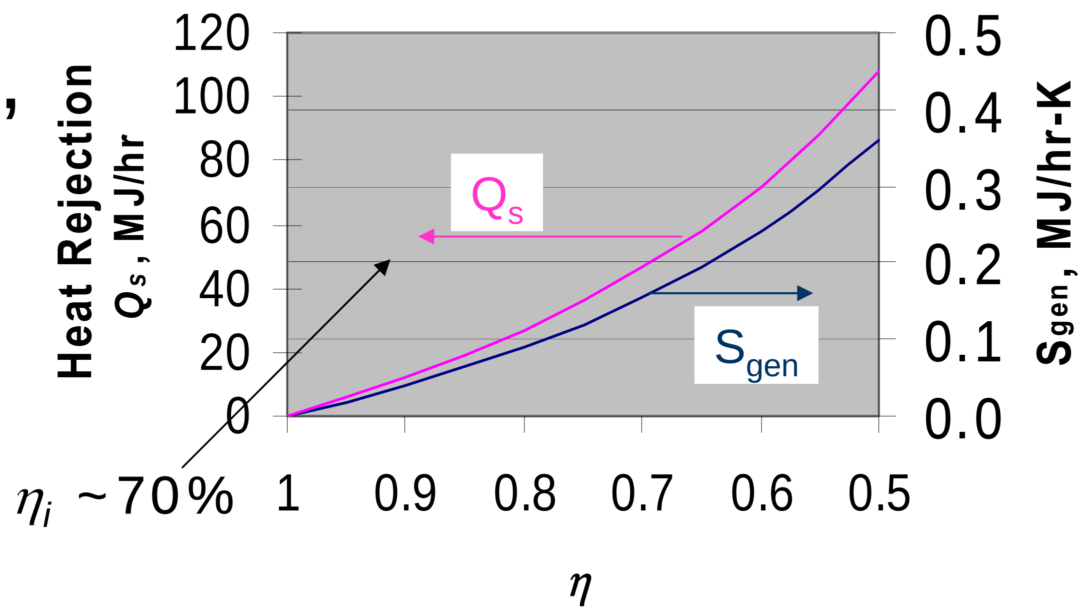
- Case: heat engine of efficiency, η_i

$$S_{gen} = \frac{W}{T_s}\left(1-\frac{1}{\eta_i}\right) = -\frac{Q_s}{T_s}$$



- For SI process,

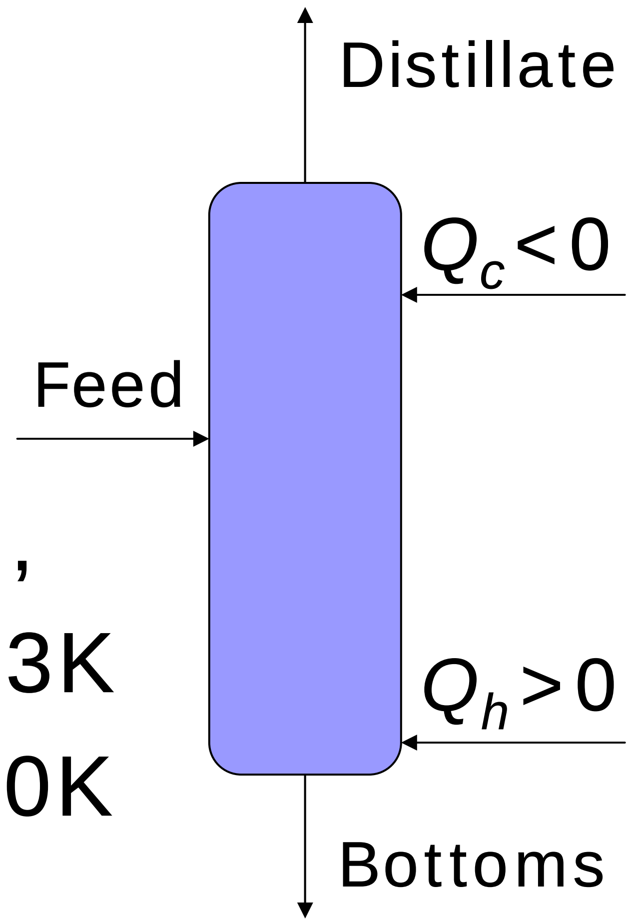
$$W \approx -30\text{kW}$$
$$= -100\text{MJ/hr}$$



TO GET A FEELING FOR S_{GEN}

- Case: S-I Distillation column

$$\dot{S}_{gen} = -\left[N \Delta s + \frac{Q_h}{T_h} + \frac{Q_c}{T_c} \right]$$



- Most efficient configuration,

Q_h = 1000 MJ/hr, T_h = 563K

Q_c = - 650 MJ/hr, T_c = 520K

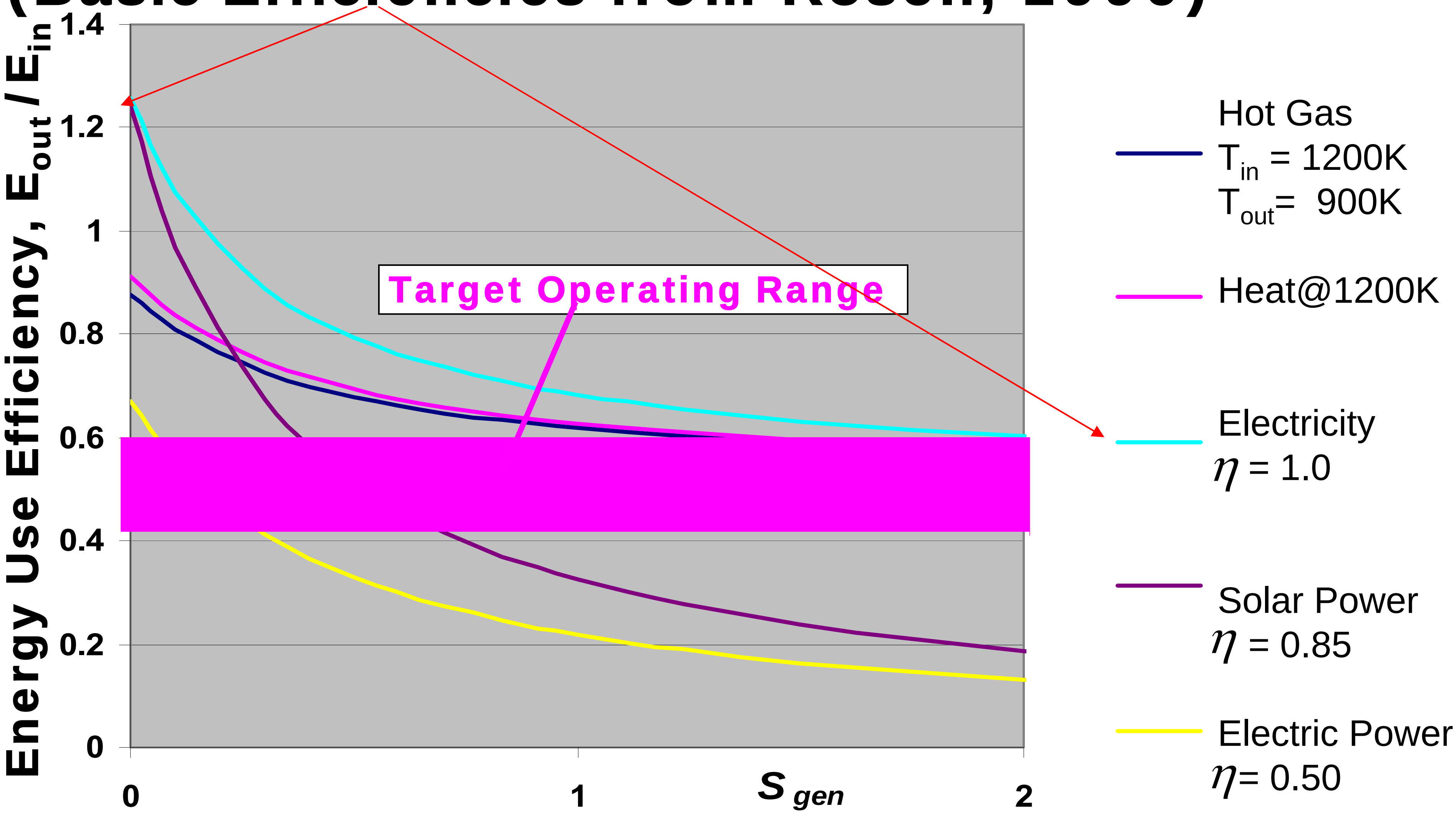
S_{gen} = 1.42 MJ/hr-K

(Current RD S_{gen} = 1.55 MJ/hr-K)

Properties from Aspen Models

PROCESS EFFICIENCIES USING VARIOUS ENERGY SOURCES

(Basic Efficiencies from Rosen, 1996)

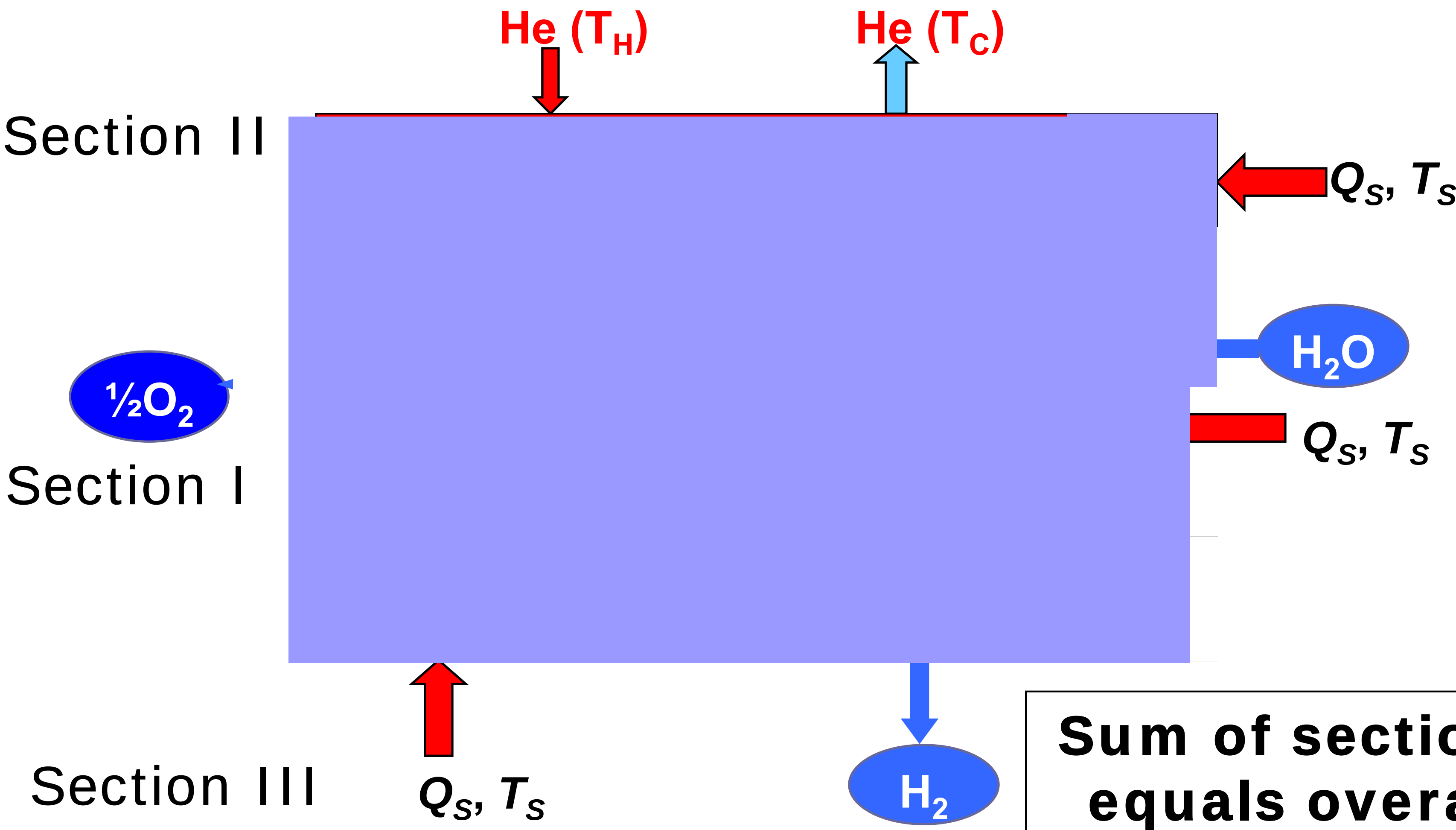


RESULTS WITH IRREVERSIBILTIES FOR WATER-SPLITTING – He FLOW

"Typical" Case: ΔT_{He} = 300K, $T_{He,in}$=1100K

S_{gen}	MJ/kmol H_2-K	0
He Flow	kmol/kmol H_2	56
Heat rejected	MJ/kmol H_2	-58
Energy Utilization Efficiency	E_{in}/E_{out}	0.86
Process Efficiency	$\Delta H_w/E_{in}$	0.83

Sections of SI Cycle

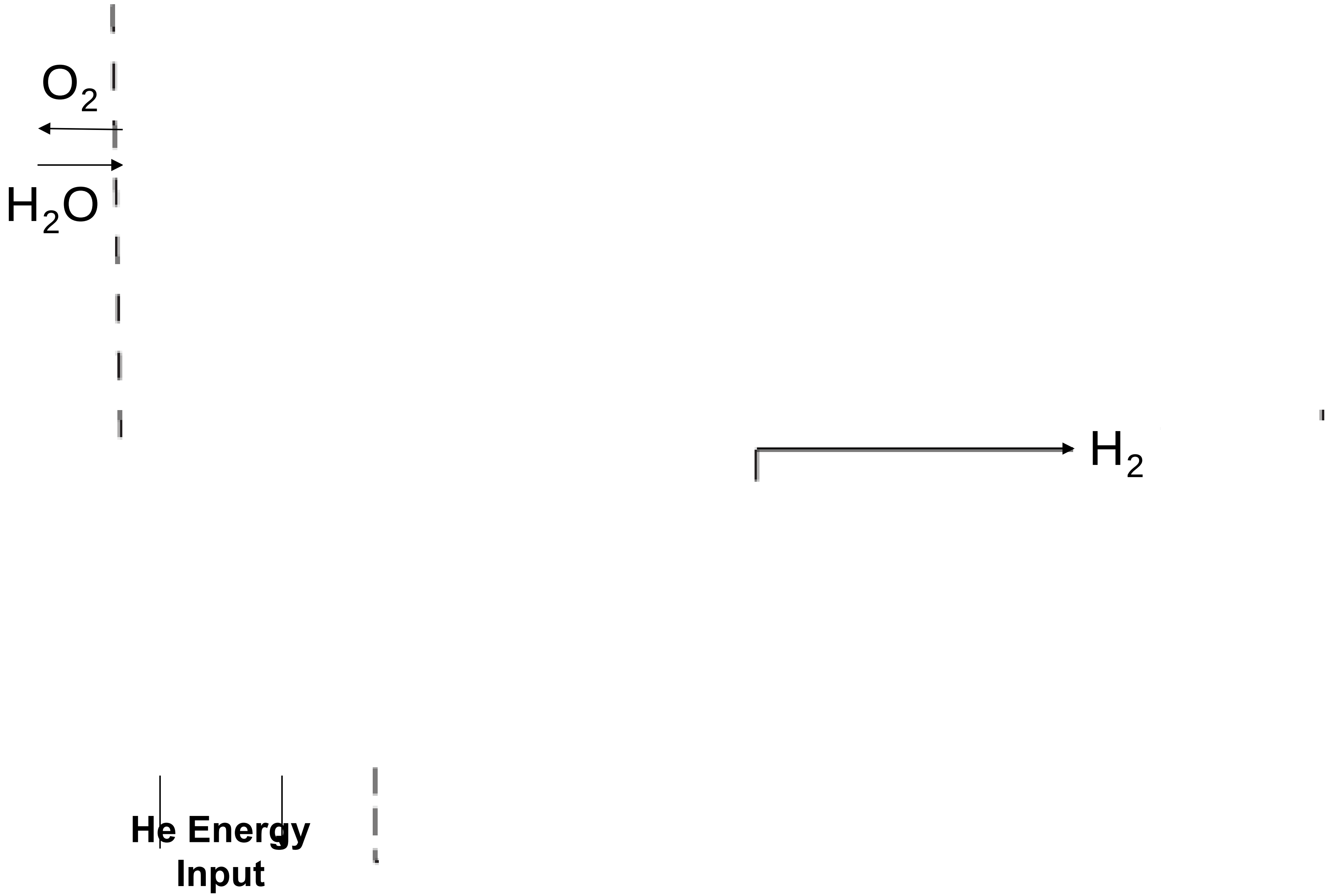


Sum of sections equals overall

Reversible Analysis → Minimum Sectional Q_i,Q_S,N_{He}

Real Analysis for Actual Q_s, S_{gen}

JAERI PROCESS (Kasahara, et al. 2003)



REVERSIBLE S-I SECTIONS

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)	$T_{\text{He In}}$ = 1200K; $T_{\text{He Out}}$ = 900K			
Overall	-	-	-57	56

REAL S-I PROCESSES

Case	S_{gen} MJ/hr-K	Q_S MJ/hr	He Flow[a] Kmol/hr
Overall	0	-46	56
Overall	1.5	-672	256

[a] $T_{\text{He In}} = 1200K$; $T_{\text{He Out}} = 900K$

*L. Brown, P. Mathias (2004); +S. Kasahara, et al. (2003)

DIFFERENT PROPERTY MODELS

h, *s* calculations with Aspen & OLI Models

GA Section I

Software	H_{in}-H_{out} MJ/hr	S_{in}-S_{out} MJ/hr-K	S_{gen} MJ/hr-K
Aspen	738	5.1	-3.12!
OLI, Inc.	395	0.8	1.23

Major differences in *h*, *s* of HI_x streams
More energy out of OLI section⇒different process
Must have S_{gen} >0; results sensitive to model!
Not clear if OLI is “true”; need to test more

CONCLUSIONS

- Model-free analysis shows:
  - Efficiency of overall process related to S_{gen}
  - For reversible sections, adding recycles leads to large internal heat flows, but unchanged overall He flow & heat rejection
  - For irreversible sections, internal heat flows further increased, He flow & heat rejection much greater
- Property model effects appear significant
  - Unphysical results ($S_{gen} < 0$) useful reliability test?
- Further analysis needed for “true efficiencies”
- Validated comparisons/decisions may require standardization of process inlets/outlets tested with several property models

[redacted]

WATER SPLITTING BALANCES

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

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

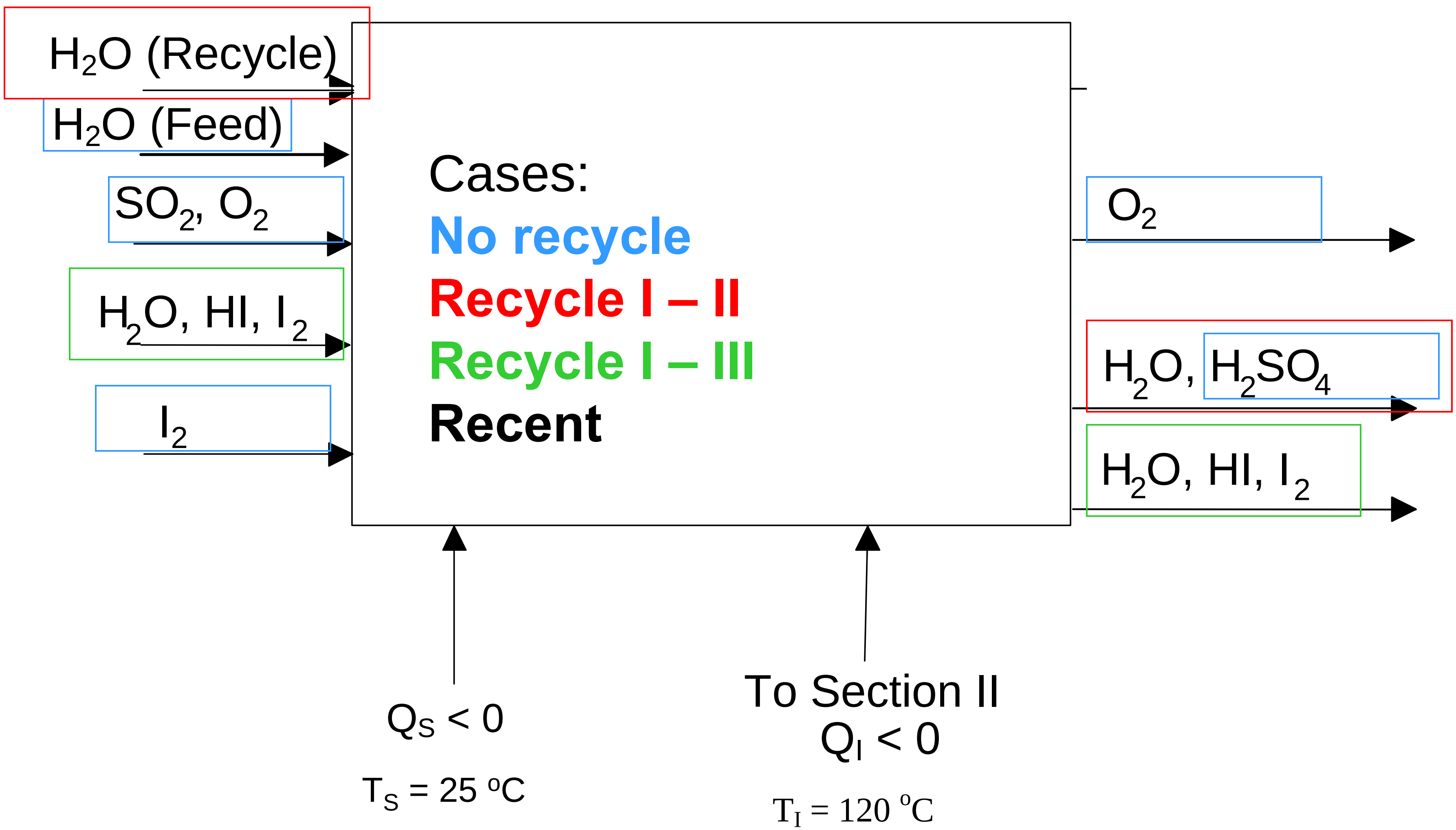
$$\dot{n}_{He\ in}(s_{He\ in} - s_{He\ out}) - \dot{n}_{H_2\ out}(s_{H_2\ out} + \frac{1}{2}s_{O_2\ out} - s_{H_2O\ in}) + \frac{\dot{Q}_s}{T_s} + S_{gen} = 0$$

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

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 $\dot{Q}_s$ & $\dot{n}_{He\,in} \Rightarrow \eta$

MATERIAL FLOWS SECTION I



EQUATIONS FOR SECTIONS

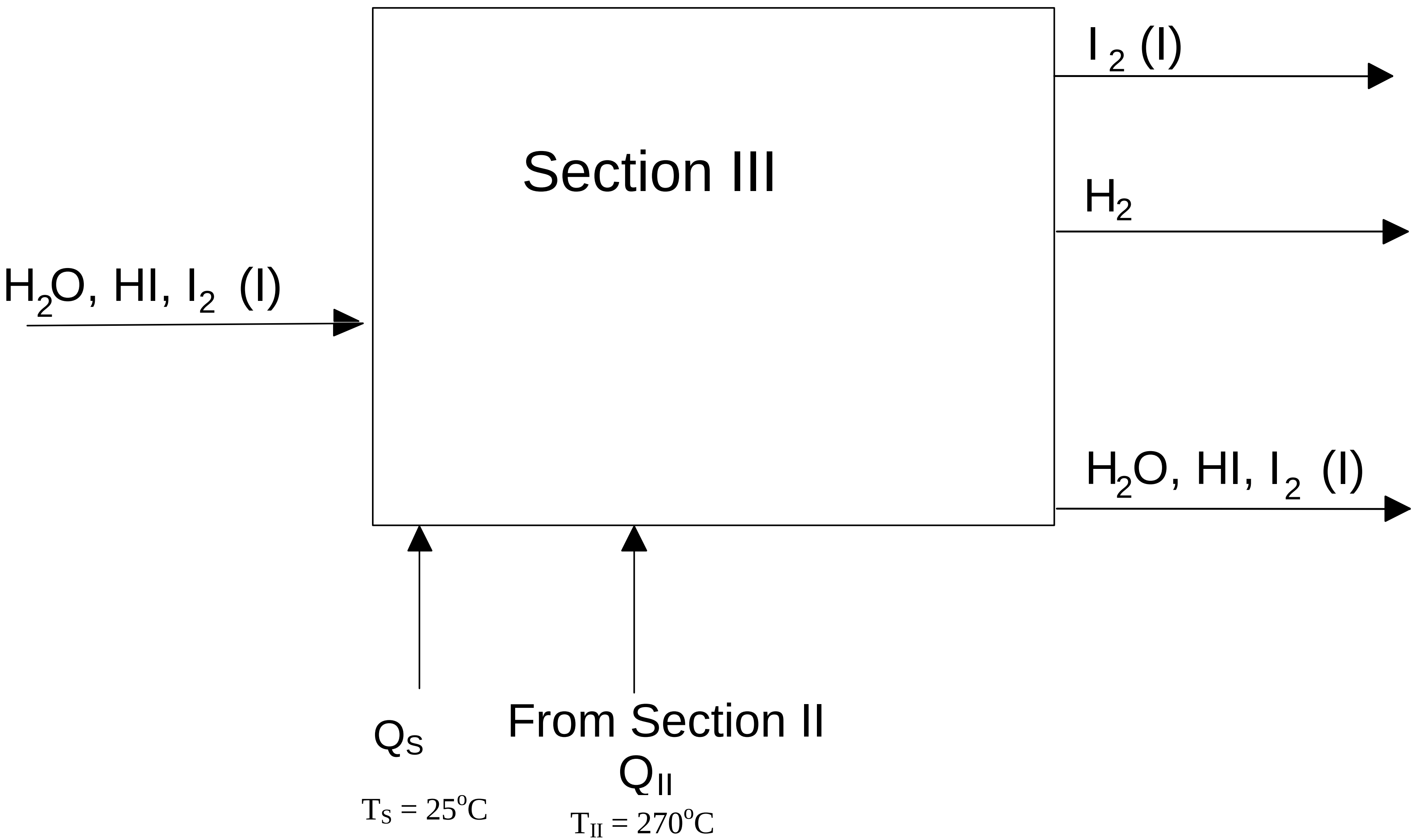
- 1^{st} Law

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

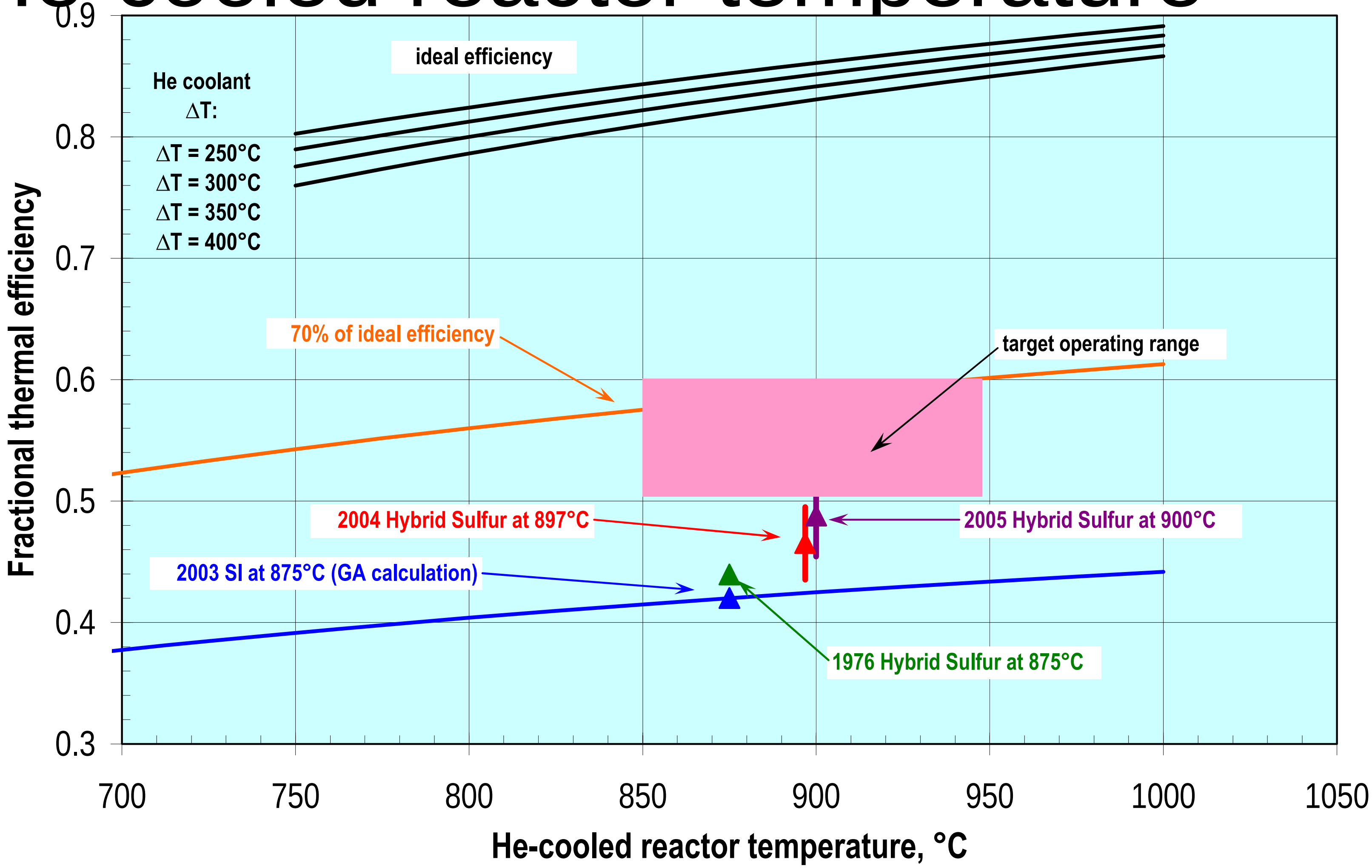
- 2^{nd} Law (reversible for $\dot{S}_{gen} = 0$)

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

MATERIAL FLOWS SECTION III



Thermal efficiency as a function of He-cooled reactor temperature



GENERAL APPROACH

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

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

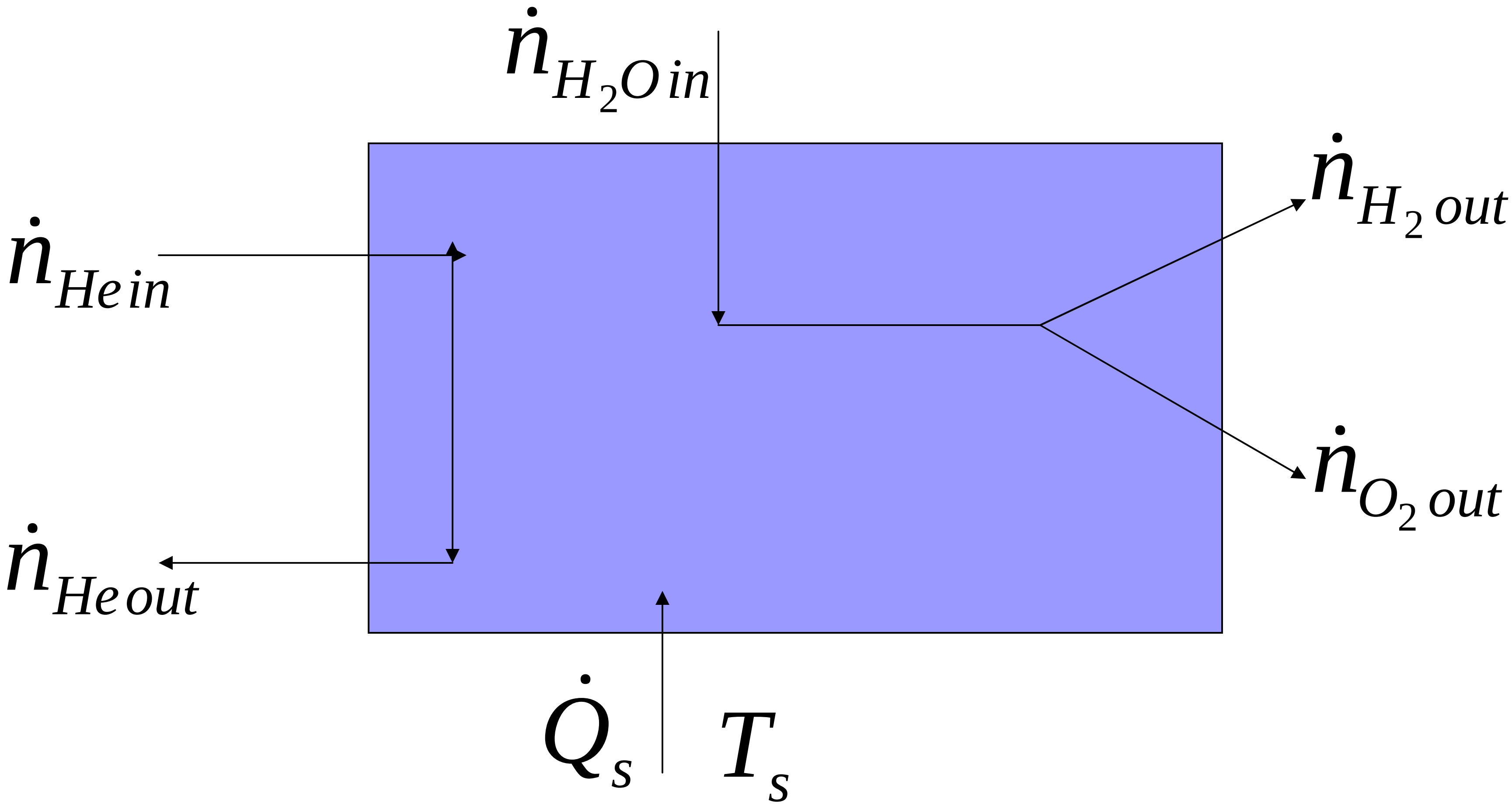
- 2nd Law (reversible for $\dot{S}_{gen} = 0$)

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

SOLVE FOR 2 VARIABLES

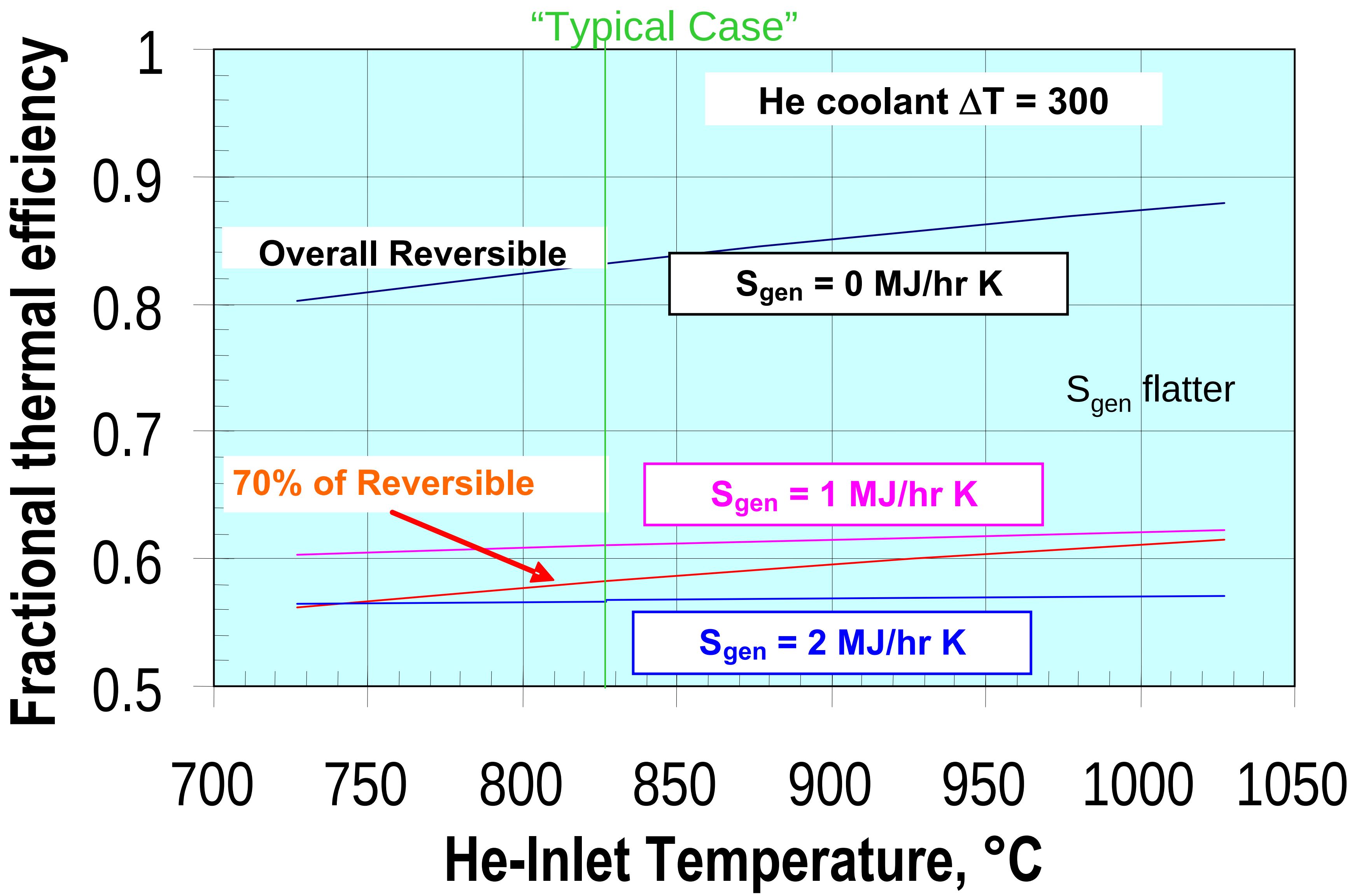
- Variables:
  - Inlet/outlet streams: T, P, $\dot{n}_i, \dot{n}_o$
  - Heat effects: $\dot{Q}_i$ & $\dot{Q}_S$
- Use property model relations for reaction & stream enthalpies, h, entropies, s
- Use 2 equations to solve for 2 variables of:
  Thermochemical water-splitting system
- For reversible compared to real, 1 condition different
- For real, what S_{gen} matches simulation results?

OVERALL WATER SPLITTING



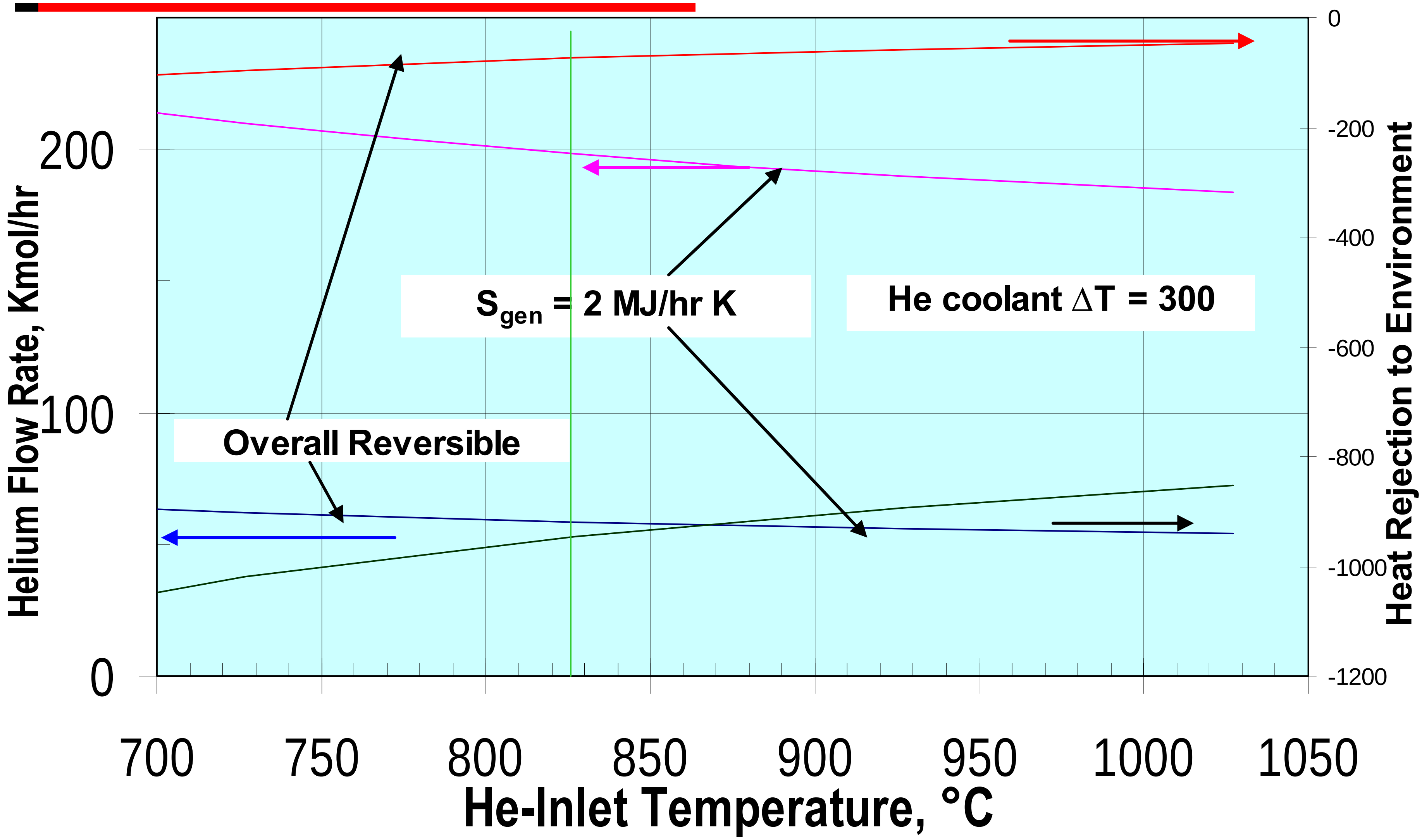
$$\dot{n}_{He\,out} = \dot{n}_{He\,in} \qquad \dot{n}_{H_2\,out} = 2\dot{n}_{O_2\,out} = \dot{n}_{H_2O\,in} = 1\,\text{kmol/hr}$$

OVERALL WATER SPLITTING

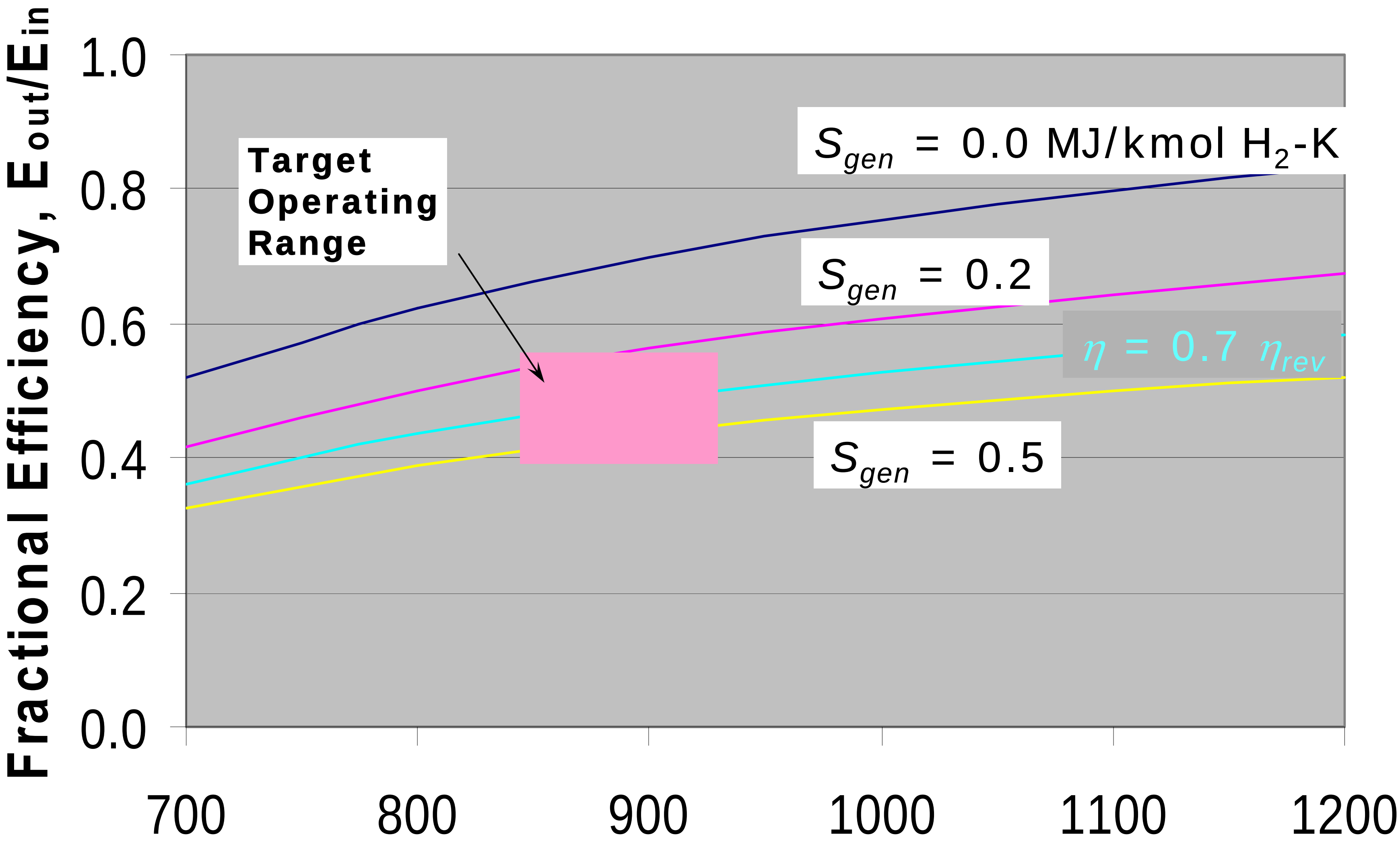


He & Heat Flows for Water-Splitting

Use a Table here



EFFICIENCY FOR NUCLEAR He



Input: $H_2O(l)$ @25^{o}C

TYPICAL GA 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°C; $T_{He\ Out}$ = 527°C				
Overall	-	-	-74	58
No Recycle	-109	-25	-74	58
Recycle I-II	-1052	25	-94	183
Recycle I-III	362	-229	-94	183
Recent	-5163	-1432	-94	183
Irreversible to Match Real Flows (S_{gen} > 0)				
No Recycle	-10(0.07)	-342(0.48)	-315	97
Recycle I-II	-757(0.24)	-342(0.48)	-384	108
Recycle I-III	362(<0)	-342(0.86)	-445	118
Recent	-757(3.58)	-342(2.69)	-982	205