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Exergetic, Environmental and Sustainability Assessment of a Fuel Cell

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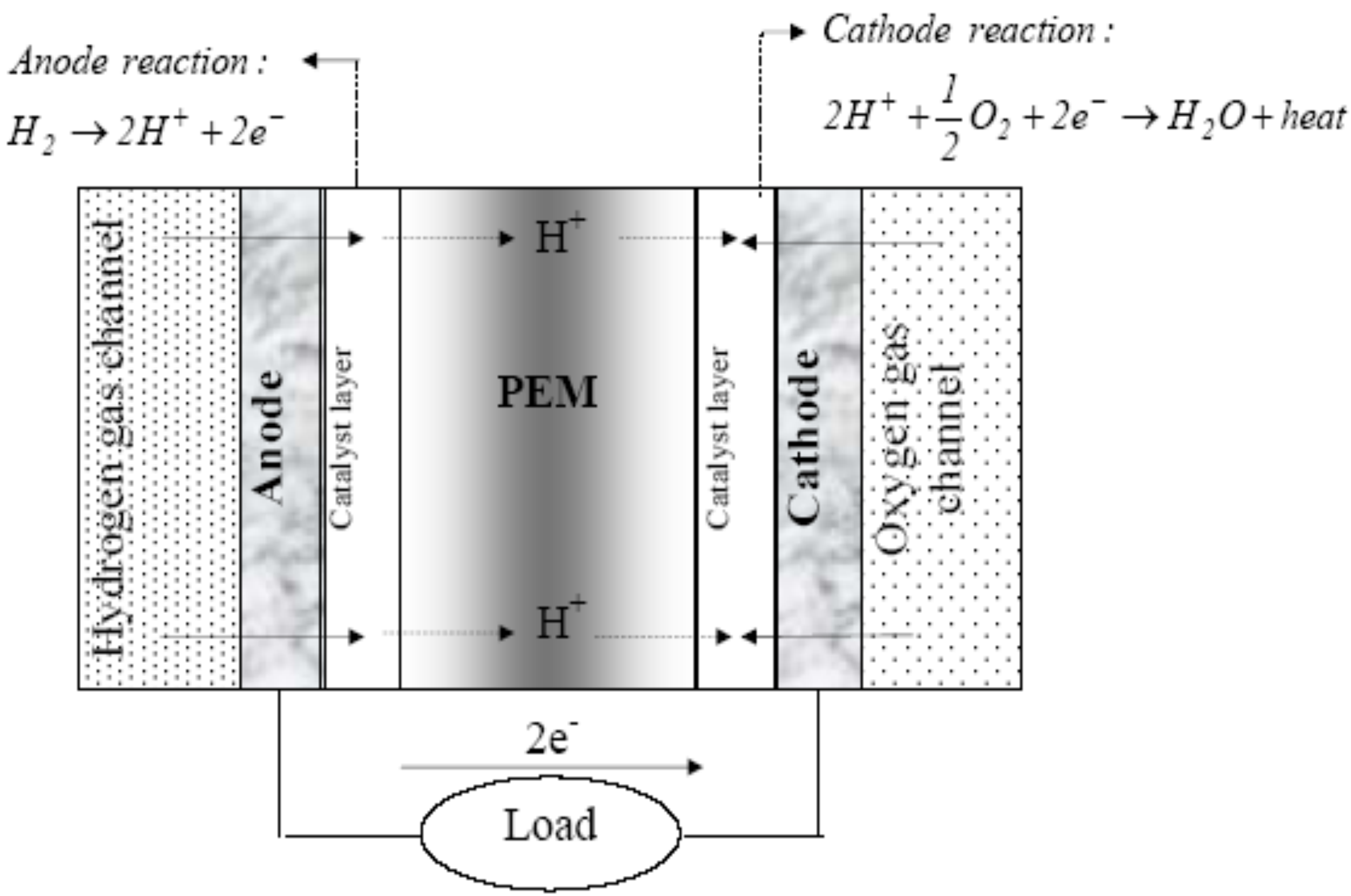
Outline

- Target of the work
- Analysis (Assumptions, process description, a PEMFC)
- Exergy analysis
- Energy sustainability indicators

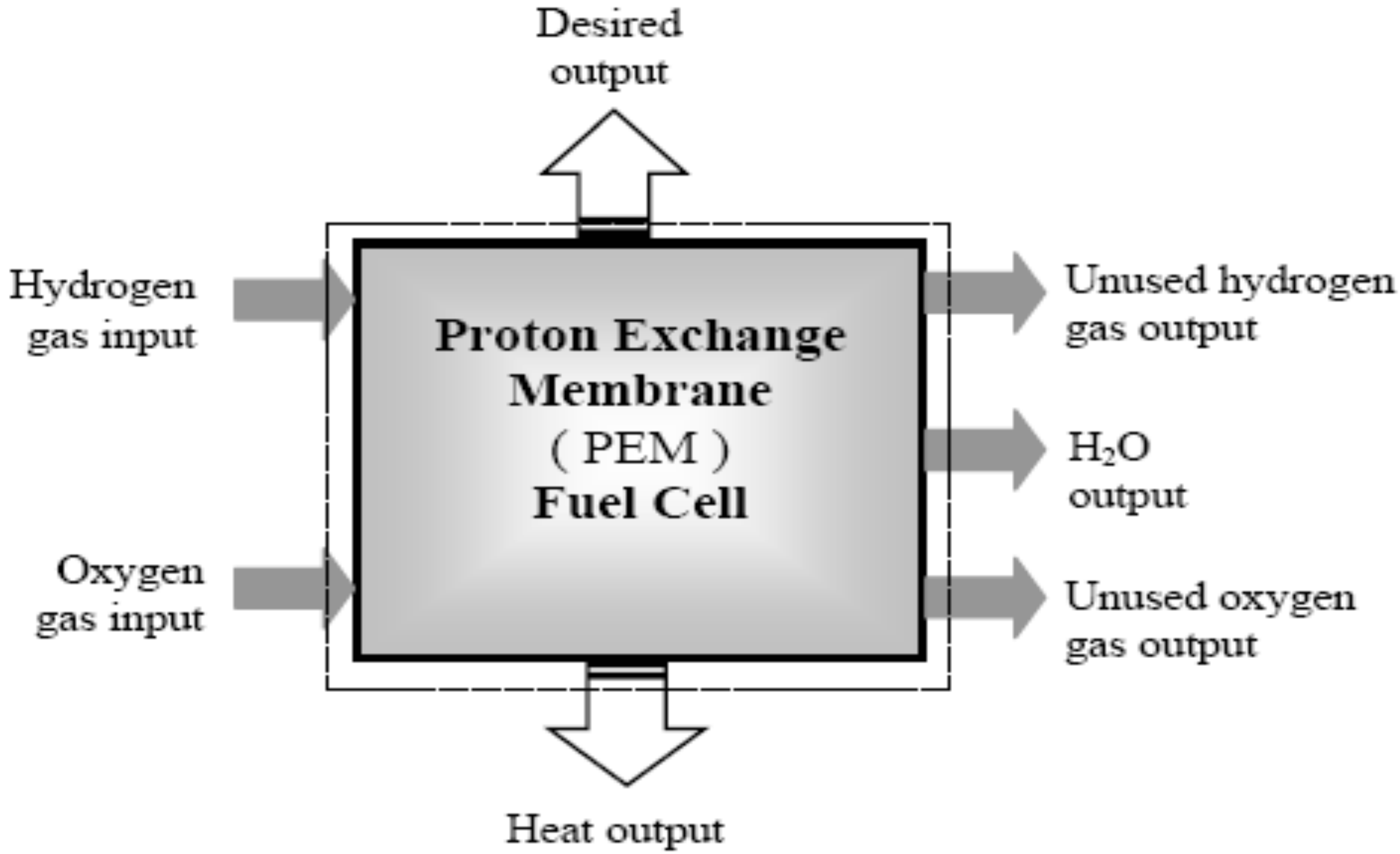
Objective

- Investigating the exergetic, environmental and sustainability aspects of a fuell cell.

General Information



a) Details of a PEM fuel cell



b) Reactants and products in a PEM fuel cell

• Analysis

• Assumptions

- Proton Exchange Membrane fuel cell is under steady-state conditions,
- Flow of reactants is steady, incompressible and laminar,
- The product water is in liquid phase,
- All gases are ideal gases,
- Kinetic and potential exergies are neglected,
- Chemical exergy values are taken from literature (Gaggioli and Petit, 1997),
- Cell temperature is taken as 323 K according to the PEM fuel cell operating conditions,
- Cell pressure is taken as 3 atm,
- Values of membrane thickness is selected as 0.016 cm,
- Current densities are 0.05-2.0 A/cm^2 with 0.05 A/cm^2 intervals,
- Dead state pressure is 1 atm and dead state temperature is 298.15 K,
- Heat loss ratio (r_{HL}) is taken as 20 %. According to Cownden *et* al. (2001), it is emphasized that 20% of total heat generated by the fuel cell is lost via convection and radiation from the fuel cell,
- The mass flow rate of the water used to humidify the oxygen and hydrogen streams is negligible. This simplification will have only negligible effects on the exergy analysis results presented subsequently because the flow rate of humidification water is small and it is at near-environmental conditions (implying its specific exergy is small) (Cownden *et* al., 2001; Dincer, 2002a).

Table 1. Constant and variable parameters for calculations

Parameter	Symbol	Unit	Value
Cell temperature	T_{fc}	K	323
Cell pressure	P	atm	3
Membrane thickness	t_{mem}	cm	0.016
Current density	I	A/cm^2	0.05-2.0
Anode stoichiometry	ζ_A	-	1.5 (Rowe and Li, 2001)
Cathode stoichiometry	ζ_C	-	3.0 (Rowe and Li, 2001)
Anode transfer coefficient	α_A	-	0.5 (Marr and Li, 1999)
Cathode transfer coefficient	α_C	-	1.0 (Marr and Li, 1999)
Universal gas constant	R	J/(mole K)	8.314
Faraday's constant	F	C/mole	96485
Dead state pressure	P_o	atm	1.0
Dead state temperature	T_o	K	298.15
Heat loss ratio	r_{HL}	-	0.2 (Cownden *et* al., 2001; Hussain *et* al., 2005)
Number of electron involved	N	-	2.0 (Barbir and Gomez, 1997)
Anode dry gas mole fraction	x_A	-	0.0 (Rowe and Li, 2001)
Cathode dry gas mole fraction	x_C	-	3.76 (Rowe and Li, 2001)

Exergy Analysis

$$ex = ex^{ph} + ex^{ch} + ex^{pt} + ex^{kn}$$

$$ex^{ph} = (h - h_o) - T_o (s - s_o)$$

$$ex = ex^{ph} + ex^{ch}$$

$$ex^{ch} = \sum_j x_j (\mu_{jo} - \mu_{joo})$$

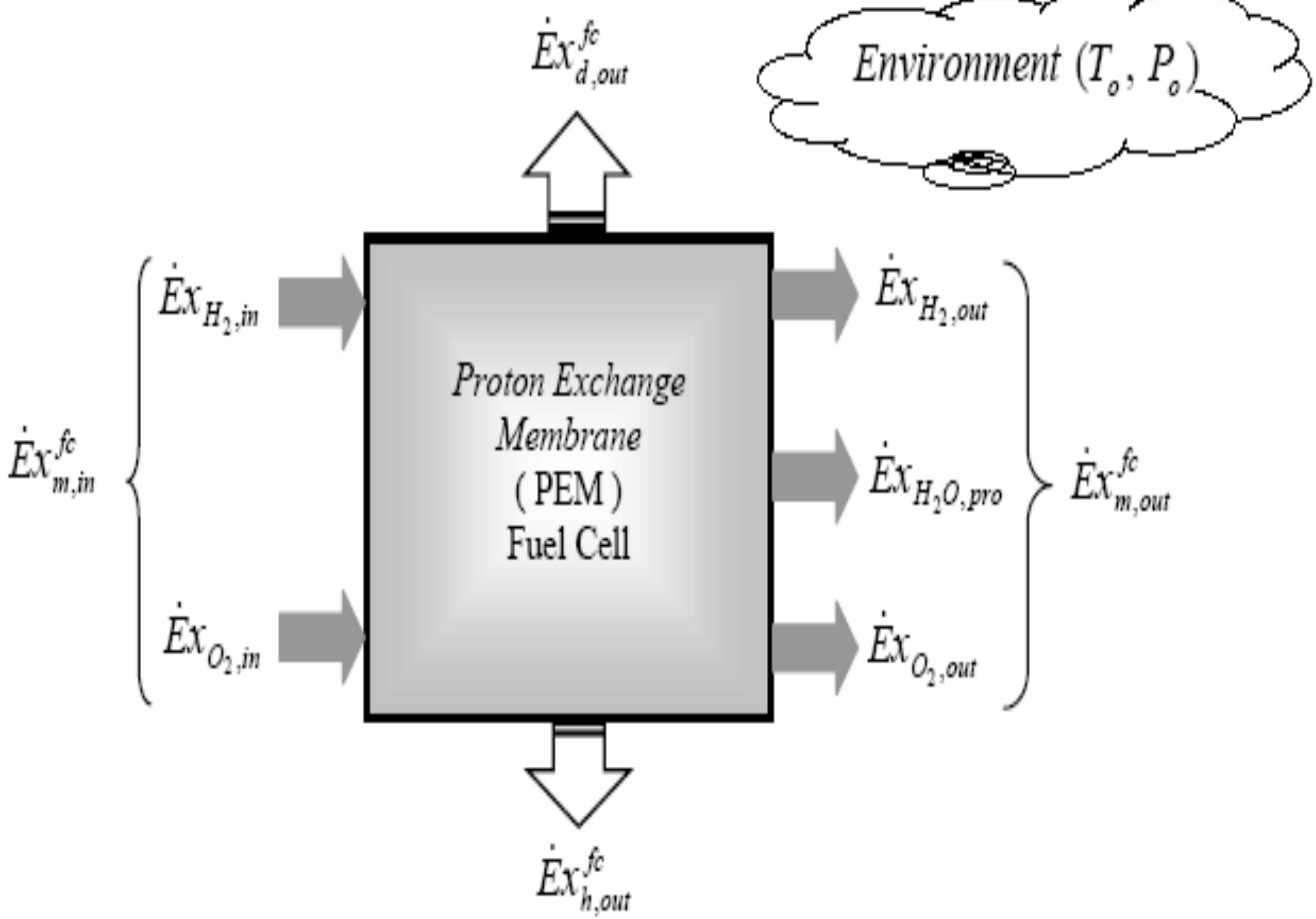


Figure 3. Schematic exergy balance diagram of Proton Exchange Membrane fuel cell

$$\sum \dot{E}x = \dot{E}x^{ch} + \dot{E}x^{ph} + \dot{E}x^{ke} + \dot{E}x^{pe} + \dot{E}x^{\cdots\cdots} \tag{5}$$

Considering Eq. (5), the general exergy balance of a PEM fuel cell can be written as

$$\begin{array}{ccccccc} \begin{pmatrix} \textit{Total} \\ \textit{exergy input} \end{pmatrix} & = & \begin{pmatrix} \textit{Total exergy of} \\ \textit{desired output} \end{pmatrix} & + & \begin{pmatrix} \textit{Total waste} \\ \textit{exergy output} \end{pmatrix} & + & \begin{pmatrix} \textit{Total exergy} \\ \textit{destruction} \end{pmatrix} \\ \sum \dot{E}x_{in}^{fc} & = & \sum \dot{E}x_{d,out}^{fc} & + & \sum \dot{E}x_{w,out}^{fc} & + & \sum \dot{E}x_{d}^{fc} \end{array} \tag{6}$$

Total Exergy Input

$$\sum \dot{E}x_{in}^{fc} = \dot{E}x_{in}^{W} + \dot{E}x_{in}^{m}$$

Where

$\dot{E}x_{in}^{W} = \dot{W}_{el}^{fc} = 0$ (no work crossing the system boundary)

$$\dot{E}x_{in}^{m} = \dot{E}x_{in}^{H_2} + \dot{E}x_{in}^{O_2}$$

Here,

- the exergy input by hydrogen gas

$$\dot{E}x_{in}^{H_2} = \dot{n}_{H_2,in} \times \left[(ex)_{H_2,in}^{ch} + (ex)_{H_2,in}^{ph} \right]$$

- the exergy input by oxygen gas

$$\dot{E}x_{in}^{O_2} = \dot{n}_{O_2,in} \times \left[(ex)_{O_2,in}^{ch} + (ex)_{O_2,in}^{ph} \right]$$

Thus, Eq. (13) can be more clearly written as

$$\dot{E}x_{in}^{m} = \dot{E}x_{in}^{H_2} + \dot{E}x_{in}^{O_2}$$

Total Exergy of Desired Output

$$\sum \dot{E}x_{d,out}^{fc} = \dot{E}x_{d,out}^{W}$$

Where

- The exergy of desired output

$$\dot{E}x_{d,out}^{W} = \dot{W}_{el}^{fc}$$

$$\dot{W}_{el}^{fc} = V(i) \times i$$

PEM fuel cell net electrical power

$$\dot{W}_{el}^{fc} = \Big[1.229 - 8.5\times 10^{-4}\,(T_{FC} - 298.15) + 4.3085\times 10^{-5}\,T_{FC}\,(\ln P_{H_2} + \frac{1}{2}\ln P_{O_2})$$

$$- \frac{\alpha_A + \alpha_C}{\alpha_A\,\alpha_C}\,\frac{R\,T_{FC}}{n\,F}\ln\frac{i}{i_0}\Big] \times i - i^2 \times t_{mem}\,[\exp(1268\,(1/303 - 1/T_{FC})$$

$$\times (0.005139\,\lambda_{mem} - 0.00326)]^{-1} - i^2 \times (\beta_1\,\frac{i}{i_{\max}})^{\beta_2}$$

where λ_{mem} defines membrane humidity. (Ay et al., 2006)

T_{fc} defines fuel cell temperature (K); σ_{mem}, membrane conductivity $(\Omega\ \mathrm{cm})^{-1}$; t_{mem}, membrane thickness, cm; β_1 and β_2, constant parameters; P_{H_2}, hydrogen partial pressure; P_{O_2}, hydrogen partial pressure; α_A, anode transfer coefficient; α_C, cathode transfer coefficient; *I*, current density, A/cm^2; i_o, exchange current density, A/cm^2; *n*, number of electron involved; $\dot{n}$, molar flow rate, mole/(cm^2-s); *F*, Faraday's constant, equal to 96485 C/mole; *R*, universal gas constant, 8.314 J/(mole-K)

Total Waste Exergy Output

$$\sum \dot{E}x^{fc}_{w,out} = \dot{E}x^{Q}_{w,out} + \dot{E}x^{H_2}_{w,out} + \dot{E}x^{O_2}_{w,out} + \dot{E}x^{H_2O}_{w,out}$$

$$\dot{E}x^{Q}_{w,out} = \dot{Q}^{fc}_{w,out} \times \left(1 - \frac{T_o}{T_{fc}}\right) \times r_{hl}$$

$$\dot{Q}^{fc}_{w,out} = \left\{T_0\left[\sum(\dot{n}\times s)_{out} - \sum(\dot{n}\times s)_{in}\right] + \dot{W}_{fc} + (\dot{n}\times ex)_{H_2,w,out} + (\dot{n}\times ex)_{O_2,w,out} + (\dot{n}\times ex)_{H_2O,w,out} - (\dot{n}\times ex)_{H_2,in} - (\dot{n}\times ex)_{O_2,in}\right\}\left(r_{HL} + (1-r_{HL})\frac{T_o}{T_{FC}}\right)^{-1}$$

-Waste exergy output by unused hydrogen gas in PEM fuel cell

$$Ex^{H_2}_{w,out} = \dot{n}_{H_2,out} \times \left[(ex)^{ch}_{H_2,out} + (ex)^{ph}_{H_2,out}\right]$$

- Waste exergy output by unused oxygen gas in PEM fuel cell

$$Ex^{O_2}_{w,out} = \dot{n}_{O_2,out} \times \left[(ex)^{ch}_{O_2,out} + (ex)^{ph}_{O_2,out}\right]$$

-Waste exergy output by water in PEM fuel cell

$$Ex^{H_2O}_{w,out} = \dot{n}_{H_2O,out} \times \left[(ex)^{ch}_{H_2O,out} + (ex)^{ph}_{H_2O,out}\right]$$

1.3.4. Total Exergy Destruction

Considering Eq. (6-22), total exergy destruction of a PEM fuel cell can be calculated as

$$\sum \dot{E}x_{d}^{fc} = \sum \dot{E}x_{in}^{m} - \sum \dot{E}x_{d,out}^{fc} - \sum \dot{E}x_{w,out}^{fc}$$

Environmental and Sustainability Aspects

i) Hydrogen Exergy Consumption Ratio in A PEMFC (r_{hec}^{fc})

ii) Exergetic Efficiency of A PEMFC (η_{ex}^{fc})

iii) Waste Exergy Ratio of A PEMFC (r_{we}^{fc})

iv) Reusable Waste Exergy Ratio of A PEMFC (r_{rw}^{fc})

v) Waste Exergy Recovery Ratio of A PEMFC (r_{rw}^{fc})

vi) Unusable Waste Exergy Ratio (r_{uw}^{fc})

vii) Exergy Destruction Factor (f_{exd}^{fc})

viii) Exergy Destruction Potential of A PEMFC (P_{exd}^{fc})

ix) Environmental Destruction Coefficient of A PEMFC (C_{ed}^{fc})

x) Exergy Exchange Factor of A PEMFC (f_{exe}^{fc})

xi) Environmental Benign Coefficient of A PEMFC (C_{eb}^{fc})

xii) Exergetic Stability Factor of A PEMFC (f_{est}^{fc})

xiii) PEMFC Impact Factor on Energy Sustainability (f_{ioes}^{fc})

$$\begin{pmatrix} \text{Total} \\ \text{exergy input} \end{pmatrix} = \begin{pmatrix} \text{Total exergy of} \\ \text{desired output} \end{pmatrix} + \begin{pmatrix} \text{Total waste} \\ \text{exergy output} \end{pmatrix} + \begin{pmatrix} \text{Total exergy} \\ \text{destruction} \end{pmatrix}$$

$$\sum \dot{E}x_{in}^{fc} = \sum \dot{E}x_{d,out}^{fc} + \sum \dot{E}x_{w,out}^{fc} + \sum \dot{E}x_{d}^{fc}$$

$$\sum \dot{E}x_{in}^{fc} = \sum \dot{E}x_{d,out}^{fc} + \sum \dot{E}x_{rw}^{fc} + \sum \dot{E}x_{uw}^{fc} + \sum \dot{E}x_{d}^{fc}$$

$$1 = \frac{\sum \dot{E}x_{d,out}^{fc}}{\sum \dot{E}x_{in}^{fc}} + \frac{\sum \dot{E}x_{rw}^{fc}}{\sum \dot{E}x_{in}^{fc}} + \frac{\sum \dot{E}x_{uw}^{fc}}{\sum \dot{E}x_{in}^{fc}} + \frac{\sum \dot{E}x_{d}^{fc}}{\sum \dot{E}x_{in}^{fc}}$$

In this equation,

$\frac{\sum \dot{E}x_{d,out}^{fc}}{\sum \dot{E}x_{in}^{fc}}$ is equal to exergetic efficiency (η_{ex}^{fc}) [26] of the process,

$\frac{\sum \dot{E}x_{d}^{fc}}{\sum \dot{E}x_{in}^{fc}}$ can be assumed as exergy destruction factor (f_{d}^{fc}) modified from Ref. [27],

$\frac{\sum \dot{E}x_{w,out}^{fc}}{\sum \dot{E}x_{in}^{fc}}$ may be assumed as waste exergy factor (f_{we}^{fc}),

$\frac{\sum \dot{E}x_{rw}^{fc}}{\sum \dot{E}x_{in}^{fc}}$ may be assumed as reusable waste exergy factor (f_{rw}^{fc})

$\frac{\sum \dot{E}x_{uw}^{fc}}{\sum \dot{E}x_{in}^{fc}}$ may be assumed as unusable waste exergy factor (f_{uw}^{fc})

Considering these expressions, Eq. (32) can be written as

$$\eta_{ex}^{fc} + f_{rw}^{fc} + f_{uw}^{fc} + f_{d}^{fc} = 1$$

1.4.2. Exergetic Efficiency of A PEMFC (η_{ex}^{fc})

In order to define the exergy efficiency of a PEM fuel cell, useful exergy output and the required exergy input should be taken into consideration. If so, the exergetic efficiency of a PEM fuel cell can be written as.

$$\eta_{ex}^{fc} = \frac{\dot{E}x_{out}^{W}}{\dot{E}x_{in}^{fc}} \tag{32}$$

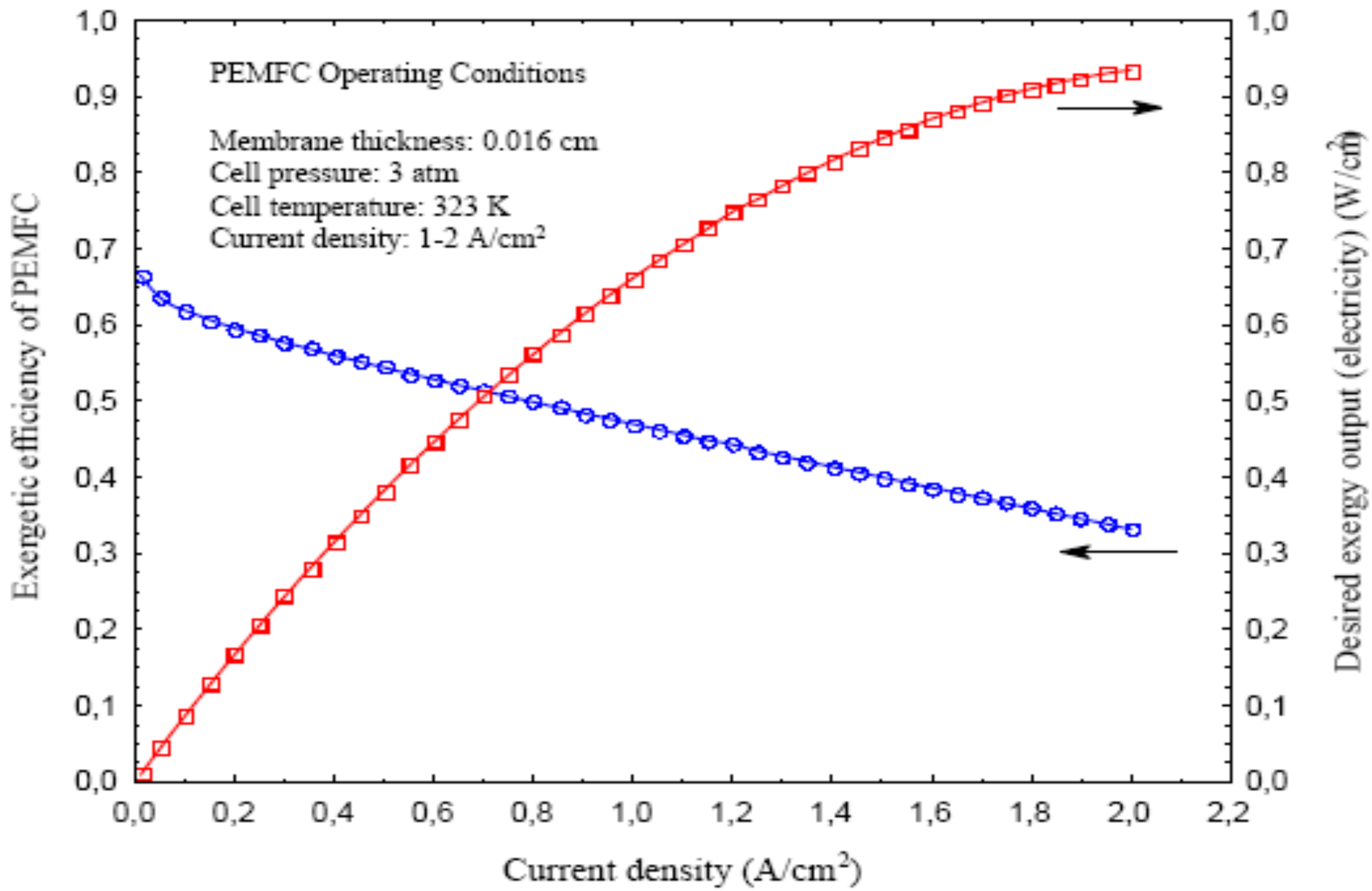


Figure 5. Exergetic efficiency and desired exergy output versus current density

Waste Exergy Ratio of A PEMFC (r_{we}^{fc})

$$\begin{pmatrix} Total\ \ waste \\ exergy\ \ output \end{pmatrix} = \left[\begin{pmatrix} \mathrm{Re}usable\ \ waste\ \ exergy \\ for\ \ the\ \ PEM\ \ \ fuel\ \ cell \end{pmatrix} + \begin{pmatrix} Unusable\ \ waste\ \ exergy \\ for\ \ the\ \ PEM\ \ \ fuel\ \ cell \end{pmatrix} \right] \tag{33}$$

Eq. (33) can be written in algebraic form as

$$\sum \dot{E}x_{w,out}^{fc} = \sum \dot{E}x_{rw}^{fc} + \sum \dot{E}x_{uw}^{fc} \tag{34}$$

Under these considerations, it may be assumed that waste exergy ratio of a PEMFC is the ratio of total waste exergy output to total exergy input. In this regard, *waste exergy factor* can be proposed as

$$\begin{pmatrix} Waste \\ exergy\ \ ratio \end{pmatrix} = \left(\frac{Total\ \ waste\ \ exergy\ \ output}{Total\ \ exergy\ \ input} \right) \tag{35}$$

Eq. (35) can be written in algebraic form as

$$r_{we}^{fc} = \left(\frac{\sum \dot{E}x_{w,out}^{fc}}{\sum \dot{E}x_{in}^{fc}} \right) = \left(\frac{\dot{E}x_{rw}^{fc} + \dot{E}x_{uw}^{fc}}{\sum \dot{E}x_{in}^{fc}} \right) \tag{36}$$

Reusable waste exergy for the PEM fuel cell

$$\dot{E}x_{rw}^{fc} = \dot{n}_{H_2,out} \times (ex)_{H_2,out}^{ch} + \dot{n}_{O_2,out} \times (ex)_{O_2,out}^{ch}$$

Unusable waste exergy for the PEM fuel cell

$$\dot{E}x_{uw}^{fc} = \dot{n}_{H_2,out} \times (ex)_{H_2,out}^{ph} + \dot{n}_{O_2,out} \times (ex)_{O_2,out}^{ph} + \dot{n}_{H_2O,out} \times (ex)_{H_2O,out} + \dot{Q}_{w,out}^{fc} \times \left(1 - \frac{T_o}{T_{fc}}\right) \times r_{hl}$$

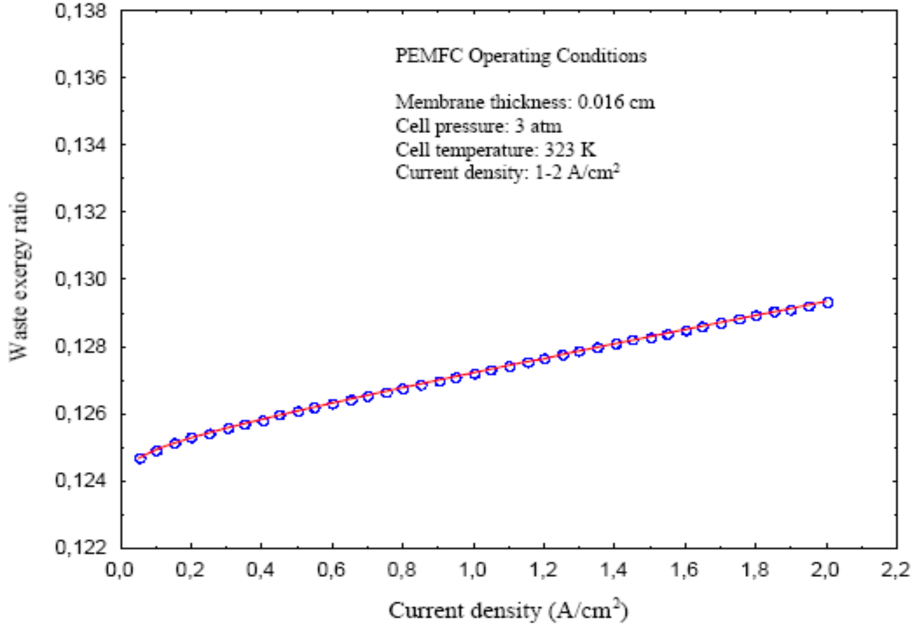


Figure 8. Waste exergy ratio versus current density

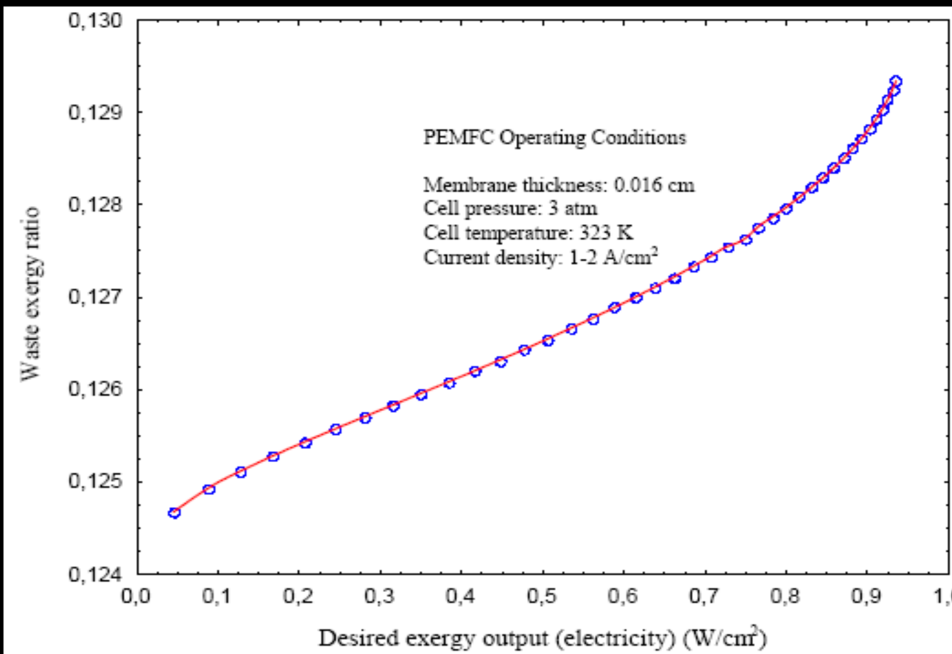


Figure 9. Waste exergy ratio versus desired exergy output

Waste Exergy Recovery Ratio of A PEMFC (r_{rw}^{fc})

$$\begin{pmatrix} Waste\ exergy \\ recovery\ ratio \end{pmatrix} = \left(\frac{\text{Reusable waste exergy}}{\text{Total waste exergy output}} \right)$$

Eq. (39) can be written as in algebraic form,

$$r_{rw}^{fc} = \left(\frac{\sum \dot{E}x_{rw}^{fc}}{\sum \dot{E}x_{w,out}^{fc}} \right) = \left(\frac{\dot{E}x_{rw}^{fc}}{\dot{E}x_{rw}^{fc} + \dot{E}x_{uw}^{fc}} \right)$$

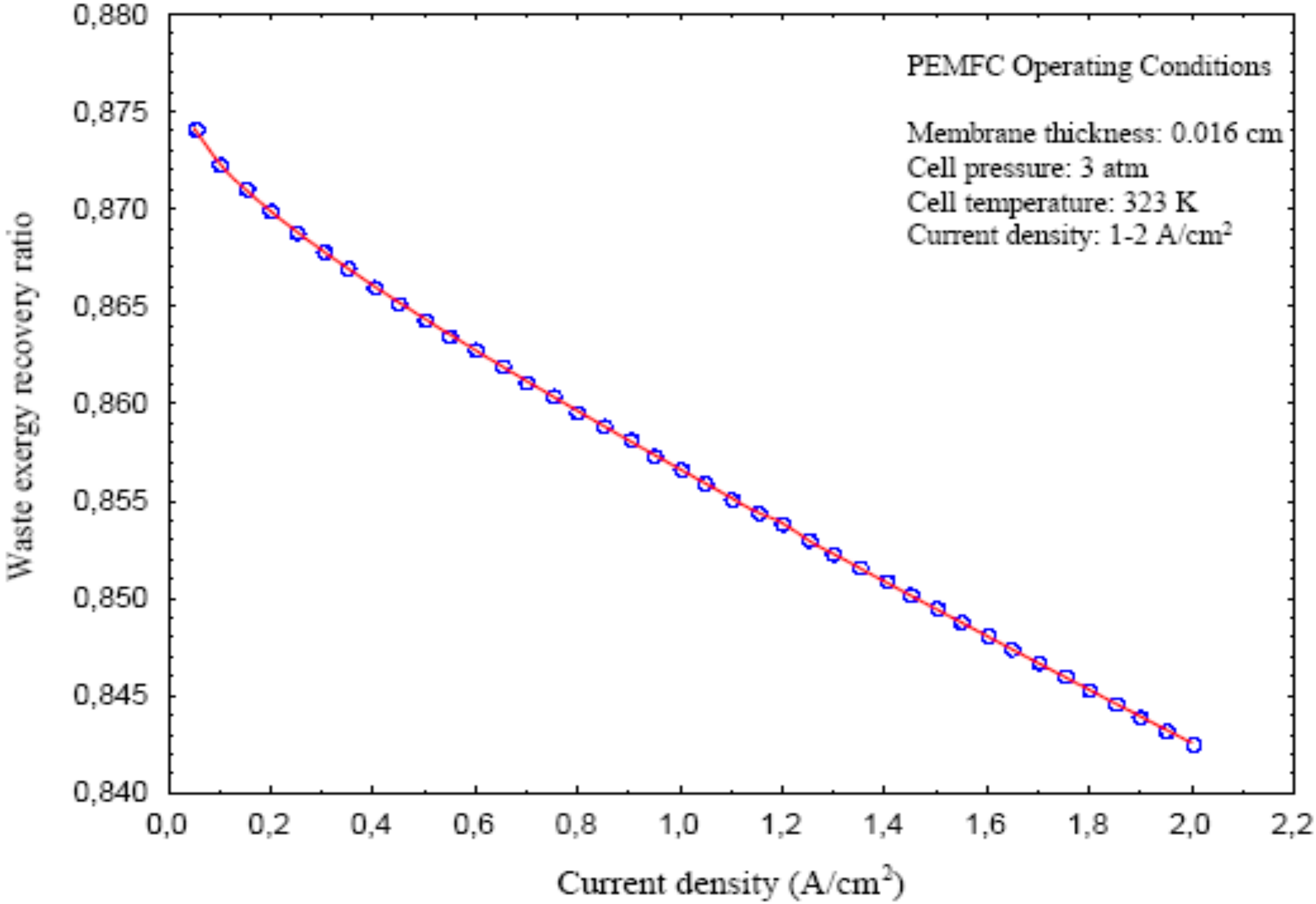


Figure 12. Waste exergy recovery ratio versus current density

Exergy Destruction Factor (f_{exd}^{fc})

$$\begin{pmatrix} Exergy \\ destruction\ \ factor \end{pmatrix} = \left(\frac{Exergy\ \ destruction}{Total\ \ exergy\ input} \right)$$

Eq. (43) can be written as in algebraic form,

$$f_{exd}^{fc} = \left(\frac{\dot{E}x_{d}^{fc}}{\dot{E}x_{in}^{fc}} \right) \qquad \text{(ranging 0 to 1)}$$

Where

f_{exd}^{fc} : Exergy destruction factor of a PEMFC

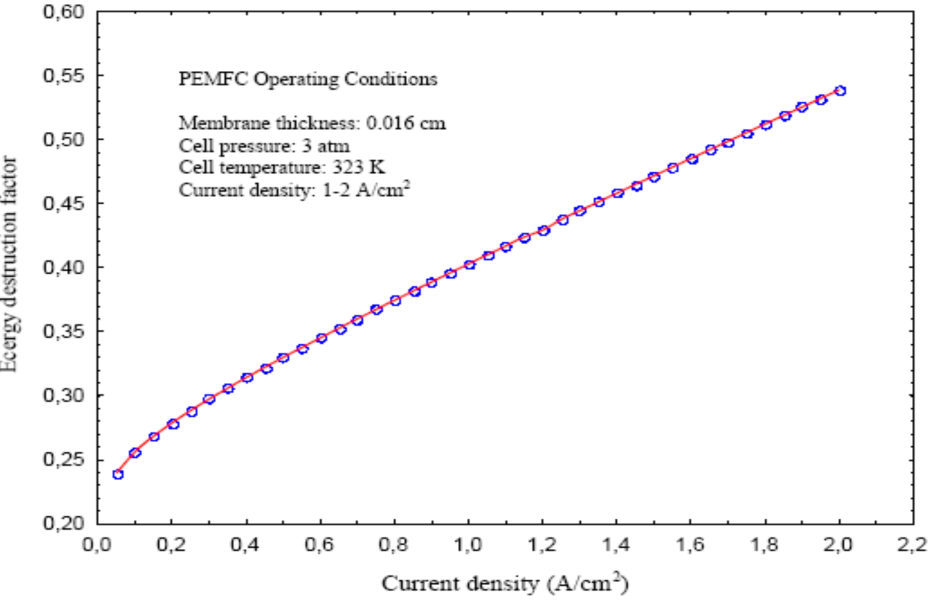


Figure 16. Exergy destruction factor versus current density

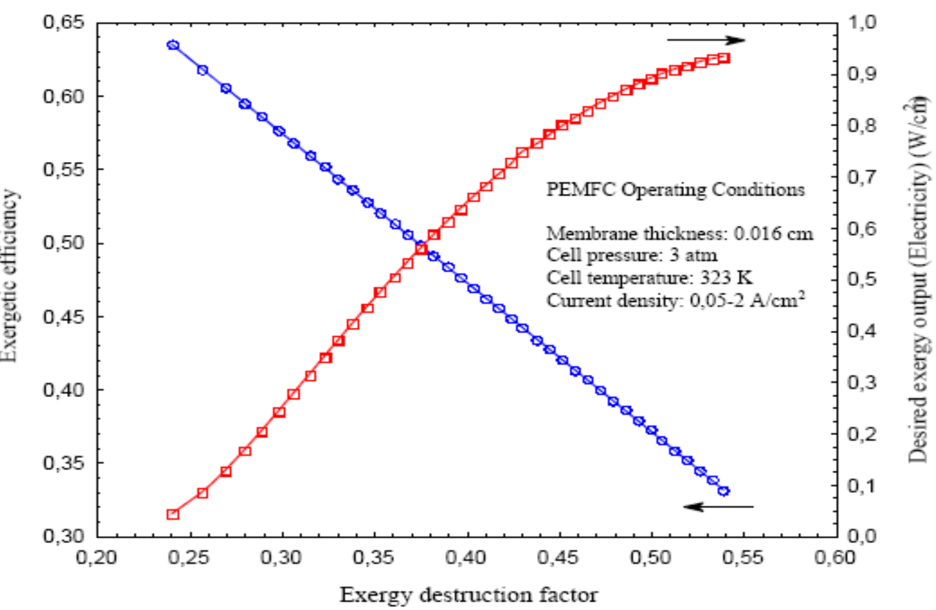


Figure 17. Exergetic efficiency and desired exergy output versus exergy destruction factor

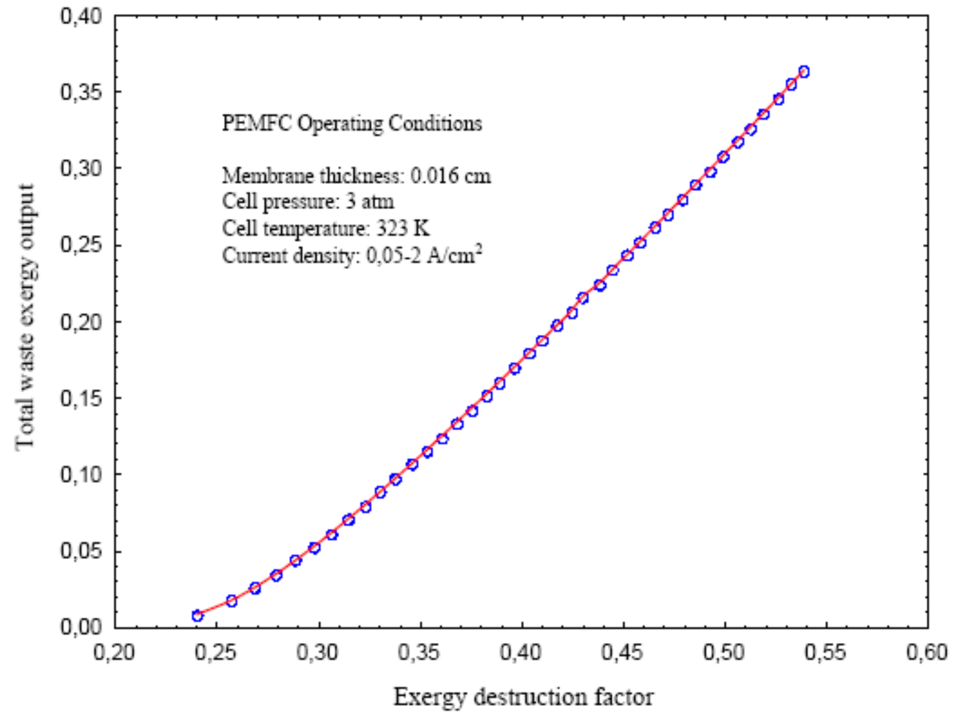


Figure 18. Total waste exergy output versus exergy destruction factor

Environmental Destruction Coefficient of A PEMFC (C_{ed}^{fc})

$$C_{ed}^{fc} = \left(\frac{P_{exd}^{fc}}{\eta_{ex}^{fc}} \right) = \left(\frac{\dot{E}x_{uw}^{fc} + \dot{E}x_{d}^{fc}}{\dot{E}x_{d,out}^{fc}} \right)$$

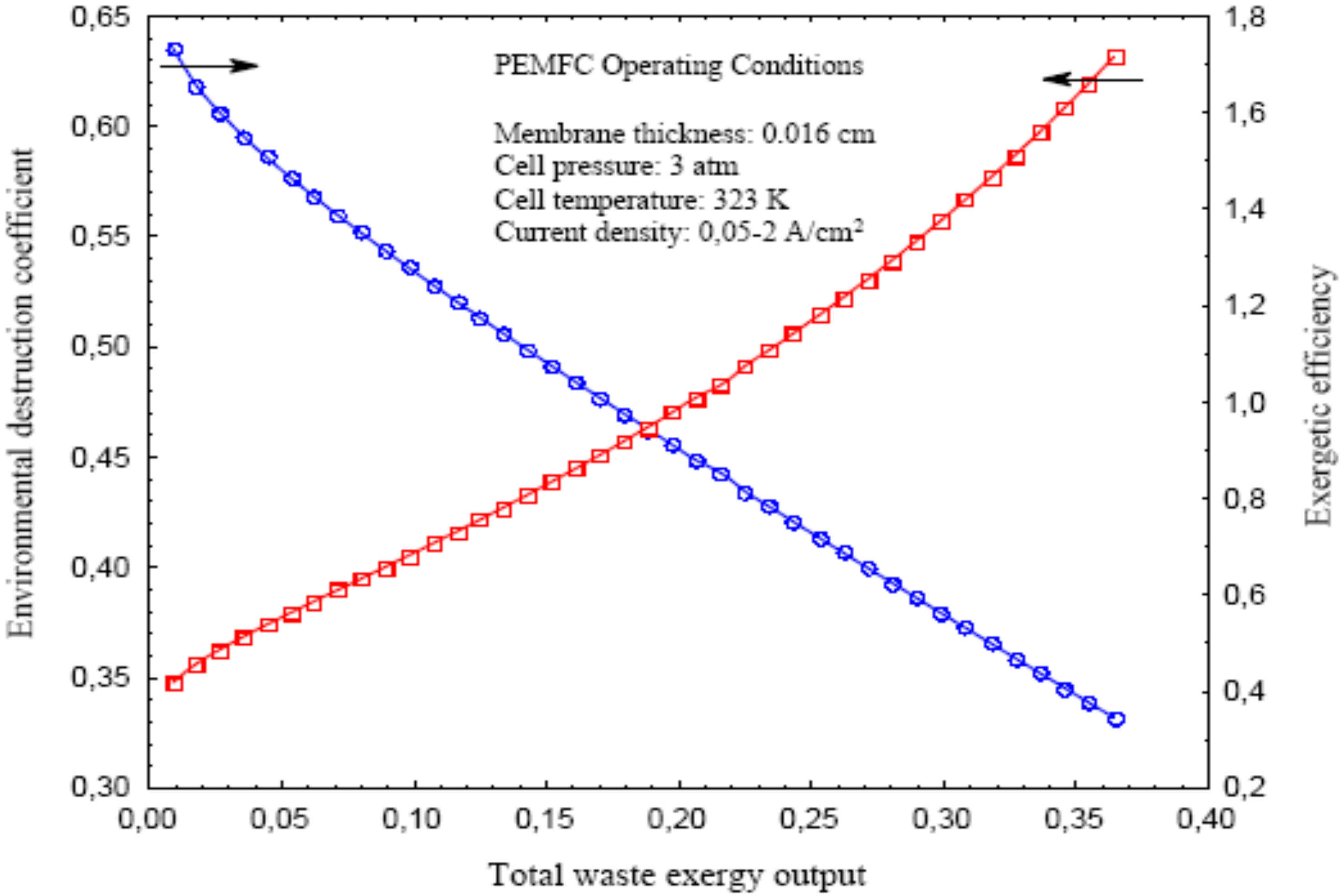


Figure 24. Environmental destruction coefficient
and exergetic efficiency versus total waste exergy output

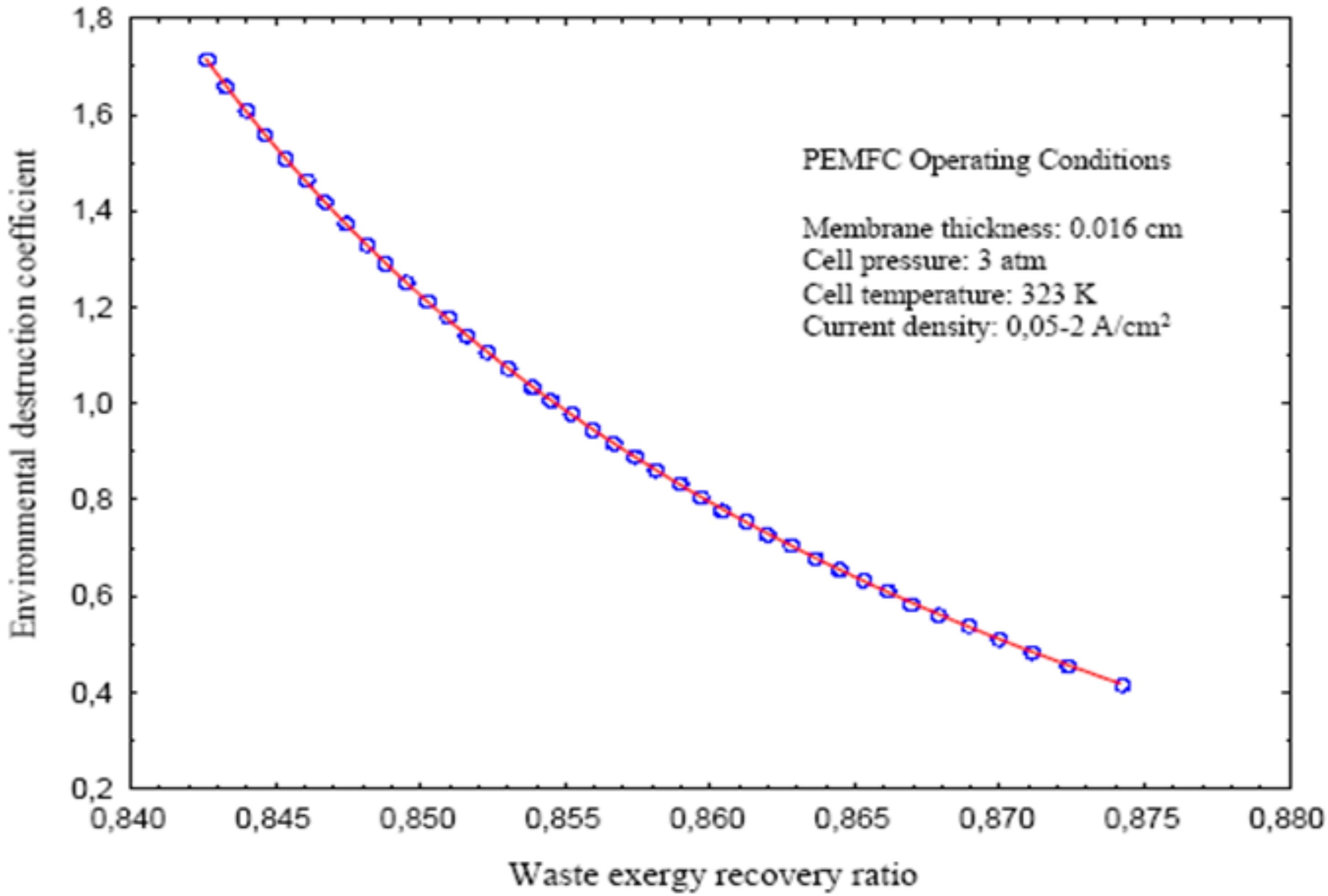


Figure 25. Environmental destruction coefficient versus waste exergy recovery ratio

Environmental Benign Coefficient of A PEMFC (C_{eb}^{fc})

$$C_{eb}^{fc} = \left[\left(\frac{\dot{E}x_{d,out}^{fc}}{\dot{E}x_{in}^{H_2}} \right) \Big/ \left(\frac{\dot{E}x_{uw}^{fc} + \dot{E}x_{d}^{fc}}{\dot{E}x_{d,out}^{fc}} \right) \right]$$

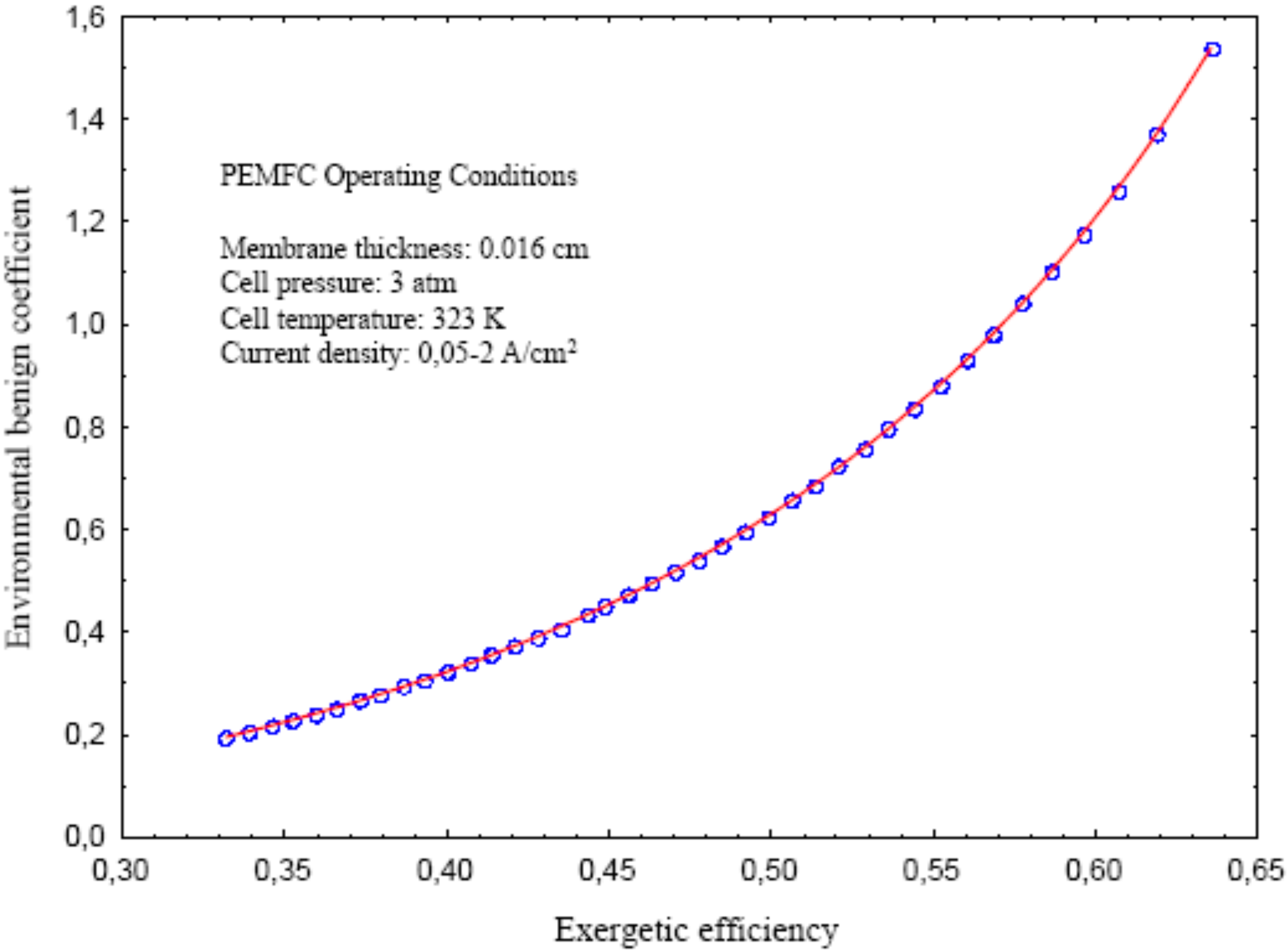


Figure 30. Environmental benign coefficient versus exergy efficiency

Exergetic Stability Factor of A PEMFC (f_{est}^{fc})

$$f_{est}^{fc} = \left(\frac{\left(\dot{E}x_{d,out}^{fc} + \dot{E}x_{w,out}^{H_2O} + \dot{E}x_{w,out}^{Q} \right)}{\left(\dot{E}x_{d,out}^{fc} + \dot{E}x_{d}^{fc} + \dot{E}x_{w,out}^{fc} \right)} \right) \quad \text{(ranging 0 to 1)}$$

Where

$$\dot{E}x_{w,out}^{fc} = \dot{E}x_{w,out}^{H_2O} + \dot{E}x_{w,out}^{Q} + \dot{E}x_{w,out}^{H_2} + \dot{E}x_{w,out}^{O_2}$$

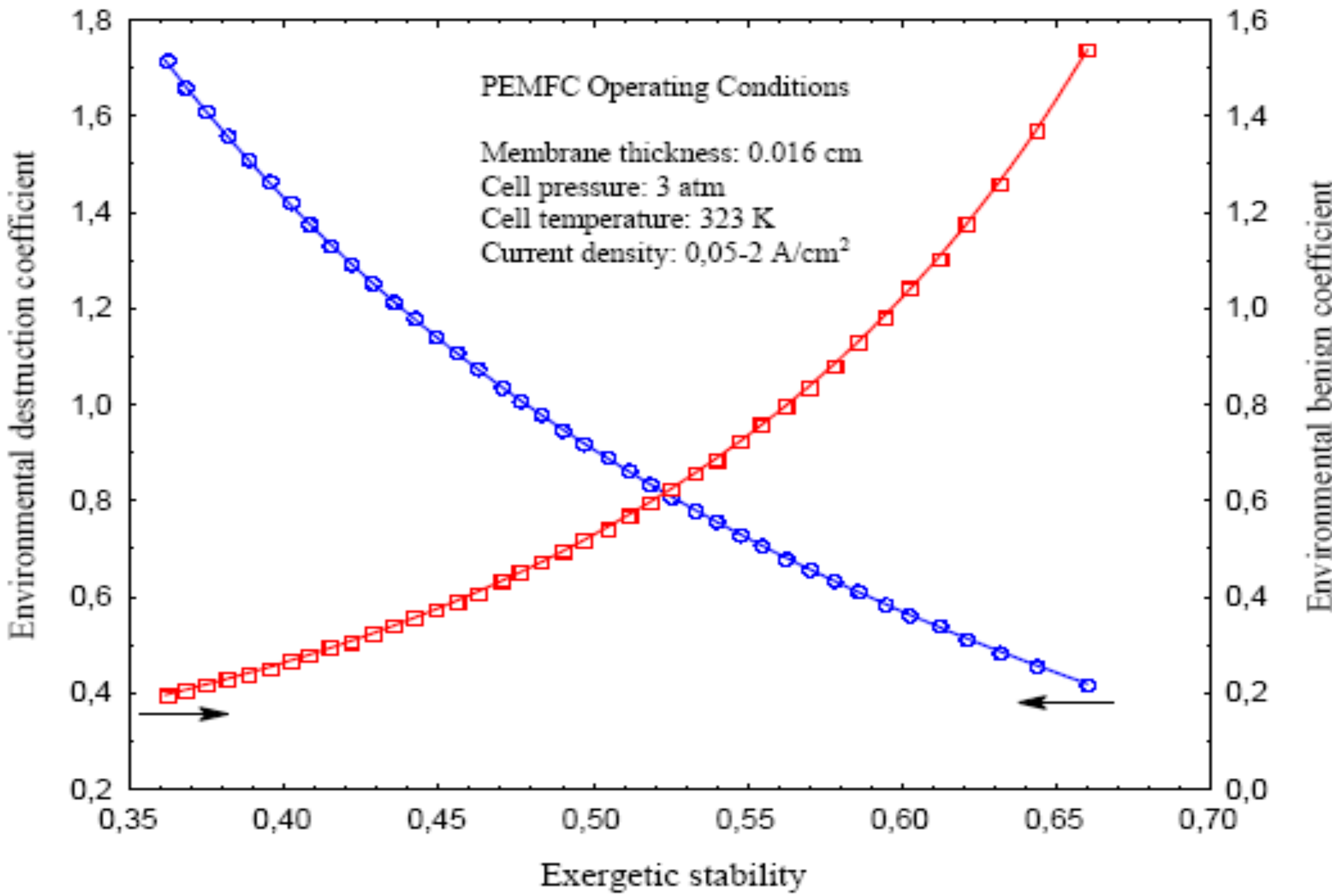


Figure 35. Environmental destruction coefficient and environmental benign coefficient versus exergetic stability

PEMFC Impact Factor on Energy Sustainability (f_{ioes}^{fc})

$$\begin{pmatrix} PEMFC\ impact\ ratio \\ on\ energy\ sustainability \end{pmatrix} = \begin{pmatrix} Hydrogen\ exergy \\ consumption\ ratio \end{pmatrix} \times \begin{pmatrix} Environmental \\ benign\ coefficient \end{pmatrix} \times \begin{pmatrix} Exergetic \\ stability\ \ factor \end{pmatrix} \quad (53)$$

Eq. (53) can be written in algebraic form as

$$r_{ioes}^{fc} = \left[\left(r_{hec}^{fc} \right) \times \left(C_{eb}^{fc} \right) \times \left(f_{est}^{fc} \right) \right] \quad (54)$$

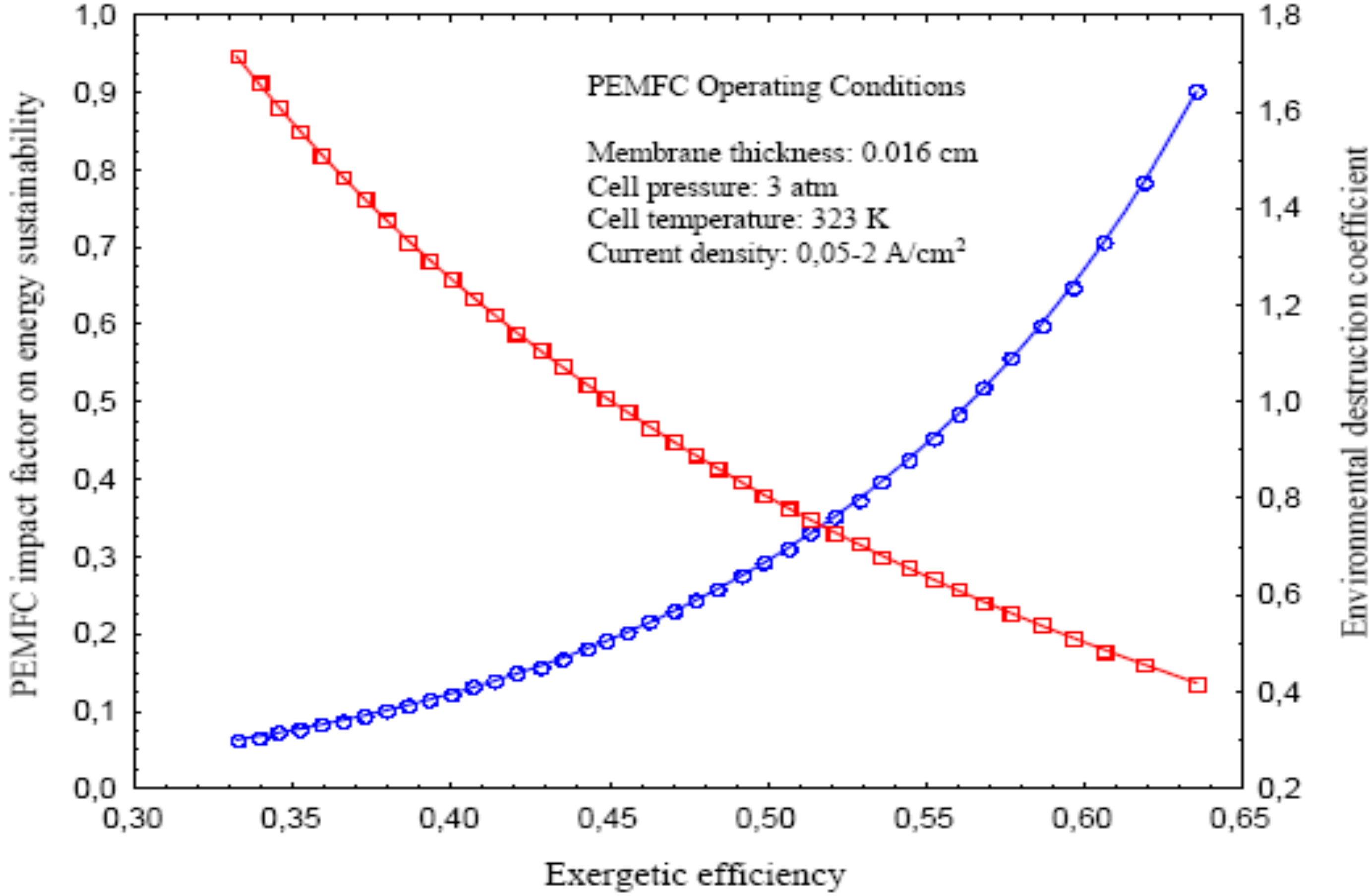


Figure 40. PEMFC impact factor on energy sustainability and environmental destruction coefficient versus exergetic efficiency

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Thank you. Have an exergetic day.

Should you wanna improve your exergetic efficiency, please follow this course by paying more attention!