Electrification of Catalytic Reactor and Distillation Processes

Chengtian Cui

Davidson School of Chemical Engineering Purdue University West Lafayette, IN, USA ctcui@purdue.edu

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Research Background



Nearly **one third** of all anthropogenic GHG emissions were from industrial activities.

Chemical industry accounts for **19%** of all industrial emissions, equivalent to **6%** of global anthropogenic GHG emissions.





Eryazici I, Ramesh N, Villa C. Electrification of the chemical industry – materials innovations for a lower carbon future. MRS Bulletin. 2021, 46: 1197-1204.

Chemical Reaction is the core of a chemical plant. **Endothermic reaction** needs energy.



- Why electrification?
- 1. Decarbonization purpose: Energy should be decarbonized to reduce the CO₂ emissions (we can use renewable electricity, e.g. wind, solar, etc), achieving the ultimate goal of carbon neutrality for human society. Transition from fossil resource based chemical production to renewable based chemical production.
- 2. **Process intensification purpose**: Improving energy efficiency and reducing energy consumption: e.g. (1) Using induction heating to directly heat the SMR catalyst active site instead of heat transferred from combustion of fossil fuel; (2) Using heat pump in distillation systems when COP is higher.



Research Background

We are interested in using direct heating measures to electrify industrial endothermic reaction.

Reasons:

 The TRL (Technology Readiness Level) is favorable.
 Suitable for retrofit.

Mallapragada DS et al. Decarbonization of the chemical industry through electrification: Barriers and opportunities. Joule. 2023, 7, 23-41.





Table 1

Electrified heating options for process industries.

Туре		Working temperature
Direct heating	Inductive heating	100–2500 °C ^a ;
	Microwave	100–1300 °C ^a ;
Indirect heating	Resistance heating	200–1800 °C ^a
	Electric arc	1200–3000 °C ^a ;
	Infrared heating	300–2600 ° C ^a
	Plasma heating	1600 °C ^b ; 2000 °C ^c
Steam generation	Electrode boiler	100–350 °C

- ^a Reference: [21].
- ^b Application for waste treatment [31].
- ^c Application for metal processing [32].

Kim JK. Studies on the conceptual design of energy recovery and utility systems for electrified chemical processes. Renewable and Sustainable Energy Review. 2022, 167, 112718.



Electrification of Chemical Reactors

US has a very large amount of shale gas.

Complete transition from fossil fuels to renewables so far is not possible.

Intermediate solutions:

Fossil resources as carbon sources.

Renewable electricity as energy sources.







Electrification of Distillation Processes



Electrification of distillation: from conventional distillation powered by steam generated from fossil fuels combustion and electricity produced via steam turbines, to electrified distillation powered by electricity sourced from the power grid or renewable power with an energy storage system, and heating demands met through power-to-heat (heat pump) technologies.



Electrification of Energy Systems



(a) Conventional systems

(b) Electrified systems

Fig. 1. Electrification for process-level energy systems.

Using electrification measures into process-level energy systems.



Kim JK. Studies on the conceptual design of energy recovery and utility systems for electrified chemical processes. Renewable and Sustainable Energy Review. 2022, 167, 112718.



- SMR is the most popular way for industrial H2 production, contributing to over 40% of the world's H2 production.
- Two steps: (I) SMR reaction; (II) Water gas shift (WGS) reaction

 $CH_{4(g)} + H_2O_{(g)} \rightleftharpoons CO_{(g)} + 3 H_{2(g)} \quad \Delta H_{rxn,298K} = 206.1 \,\text{kJ/mol} \qquad (I)$ $CO_{(g)} + H_2O_{(g)} \rightleftharpoons CO_{2(g)} + H_{2(g)} \quad \Delta H_{rxn,298K} = -41.15 \,\text{kJ/mol} \qquad (II)$

• Overall reaction (highly endothermic)

$$CH_{4(g)} + 2H_2O_{(g)} \rightleftharpoons CO_{2(g)} + 4H_{2(g)} \quad \Delta H_{rxn,298K} = 164.9 \,\text{kJ/mol} \quad (III)$$



• The intrinsic SMR reaction using a LHHW mechanism can be established as:

$$CH_{4(g)} + H_2O_{(g)} \rightleftharpoons CO_{(g)} + 3H_{2(g)} \quad \Delta H_{rxn,298K} = 206.1 \, \text{kJ/mol} \quad (I)$$

$$R_{1} = \frac{k_{1}}{P_{\rm H_{2}}^{2.5}} \left(P_{\rm CH_{4}} P_{\rm H_{2}O} - \frac{P_{\rm H_{2}}^{3} P_{\rm CO}}{K_{1}} \right) \left(\frac{1}{\rm DEN^{2}} \right) \quad \left[\frac{kmol}{kg_{cat} \cdot h} \right]$$
(A1)

$$CO_{(g)} + H_2O_{(g)} \rightleftharpoons CO_{2(g)} + H_{2(g)} \quad \Delta H_{rxn,298K} = -41.15 \, kJ/mol \quad (II)$$

$$R_2 = \frac{k_2}{P_{H_2}} \left(P_{CO} P_{H_2O} - \frac{P_{H_2} P_{CO_2}}{K_2} \right) \left(\frac{1}{\text{DEN}^2} \right) \quad \left[\frac{kmol}{kg_{cat} \cdot h} \right]$$
(A2)

 $CH_{4(g)} + 2 H_2 O_{(g)} \rightleftharpoons CO_{2(g)} + 4 H_{2(g)} \quad \Delta H_{rxn,298K} = 164.9 \text{ kJ/mol} \quad (III)$ $R_3 = \frac{k_3}{P_{H_2}^{3.5}} \left(P_{CH_4} P_{H_2O}^2 - \frac{P_{H_2}^4 P_{CO_2}}{K_3} \right) \left(\frac{1}{\text{DEN}^2} \right) \quad \left[\frac{kmol}{kg_{cat} \cdot h} \right] \quad (A3)$



Parameter	Value
L (m)	12
d_t (m)	0.1
d_p (m)	0.01
$ ho_p~({ m kg/m^3})$	2355.2
$C_{p,p} \left(\mathbf{J} \cdot \mathbf{kg}^{-1} \cdot \mathbf{K}^{-1} \right)$	950
$\lambda_p \; (\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1})$	0.3489
T_0 (K)	793.15
P_0 (bar)	25.7
$F_{\mathrm{CH}_{4},0} \; (\mathrm{kmol} \cdot \mathrm{h}^{-1})$	5.17
$F_{\rm CO,0} \; (\rm kmol \cdot h^{-1})$	0
$F_{\rm CO_{2},0} \; (\rm kmol \cdot h^{-1})$	0.29
$F_{\mathrm{H}_{2},0} \; (\mathrm{kmol} \cdot \mathrm{h}^{-1})$	0.63
$F_{\mathrm{H}_{2}\mathrm{O},0} \; (\mathrm{kmol} \cdot \mathrm{h}^{-1})$	17.35
$F_{\rm N_2,0} \; (\rm kmol \cdot h^{-1})$	0.85







• We developed some basic SMR models to understand the reactor design.





- 1D pseudo-homogeneous model (M1)
- Bulk gas material balance:

$$\varepsilon_b \frac{\partial C_i(z)}{\partial t} + \frac{\partial [C_i(z)U_z(z)]}{\partial z} = (1 - \varepsilon_b)\rho_p \sum \eta_j R_j(z)\nu_{ij} \quad \forall z \in (0, L)$$

• Bulk gas energy balance:

$$[(1-\varepsilon_b)\rho_p C_{p,p} + \varepsilon_b \rho_g(z)C_{p,g}(z)]\frac{\partial T(z)}{\partial t} + \rho_g(z)C_{p,g}(z)U_z(z)\frac{\partial T(z)}{\partial z}$$
$$= \frac{4U(z)}{d_t}[T_w(z) - T(z)] + (1-\varepsilon_b)\rho_p\sum \eta_j R_j(z)[-\Delta H_{rxn,j}(z)] \quad \forall z \in (0,L)$$

• Bulk gas momentum balance (Ergun eqn.):

$$\frac{\partial P(z)}{\partial z} = -\frac{G(z)}{\rho_g(z)d_p} \left(\frac{1-\varepsilon_b}{\varepsilon_b^3}\right) \left[150(1-\varepsilon_b)\frac{\mu_g(z)}{d_p} + 1.75G(z)\right]$$







- 1D pseudo-homogeneous model + axial mixing (M2)
- Bulk gas material balance:

$$\varepsilon_b \frac{\partial C_i(z)}{\partial t} + \frac{\partial [C_i(z)U_z(z)]}{\partial z} = \varepsilon_b \mathcal{D}^e_{i,z}(z) \frac{\partial^2 C_i(z)}{\partial z^2} + (1 - \varepsilon_b)\rho_p \sum \eta_j R_j(z)\nu_{ij} \quad \forall z \in (0, L)$$

- Bulk gas energy balance:
 $$\begin{split} & [(1-\varepsilon_b)\rho_p C_{p,p} + \varepsilon_b \rho_g(z) C_{p,g}(z)] \frac{\partial T(z)}{\partial t} + \rho_g(z) C_{p,g}(z) U_z(z) \frac{\partial T(z)}{\partial z} \\ & = \frac{4U(z)}{d_t} [T_w(z) T(z)] + \sum \left[\varepsilon_b \mathcal{D}^e_{i,z}(z) \frac{\partial C_i(z)}{\partial z} C_{p,i}(z) \right] \frac{\partial T(z)}{\partial z} \\ & + \lambda^e_z(z) \frac{\partial^2 T(z)}{\partial z^2} + (1-\varepsilon_b) \rho_p \sum \eta_j R_j(z) [-\Delta H_{rxn,j}(z)] \quad \forall z \in (0,L) \end{split}$$
- Bulk gas momentum balance (Ergun eqn.):

$$\frac{\partial P(z)}{\partial z} = -\frac{G(z)}{\rho_g(z)d_p} \left(\frac{1-\varepsilon_b}{\varepsilon_b^3}\right) \left[150(1-\varepsilon_b)\frac{\mu_g(z)}{d_p} + 1.75G(z)\right]$$









- 1D heterogeneous model (M3) = (M1) + interfacial gradients
- Bulk gas material and energy balances:

$$\varepsilon_b \frac{\partial C_i(z)}{\partial t} + \frac{\partial [C_i(z)U_z(z)]}{\partial z} = a_v k_{i,gp}(z) \left[C_{i,s}(z) - C_i(z) \right] \quad \forall z \in (0,L) \quad (20)$$

$$\varepsilon_b \rho_g(z) C_{p,g}(z) \frac{\partial T(z)}{\partial t} + \rho_g(z) C_{p,g}(z) U_z(z) \frac{\partial T(z)}{\partial z} = \frac{4U(z)}{d_t} [T_w(z) - T(z)] + a_v h_{gp}(z) [T_s(z) - T(z)] \quad \forall z \in (0, L)$$

$$(21)$$

• Catalyst material and energy:
$$\frac{\partial C_{i,s}(z)}{\partial t} = (1 - \varepsilon_p)\rho_p \sum \eta_j R_{j,s}(z)\nu_{ij} - a_v k_{i,gp}(z) \left[C_{i,s}(z) - C_i(z)\right] \quad \forall z \in (0,L)$$
(22)

$$\left[\varepsilon_{p}\rho_{g}C_{p,g,s}(z) + (1-\varepsilon_{p})\rho_{p}C_{p,p}\right]\frac{\partial T_{s}(z)}{\partial t}$$

$$= (1-\varepsilon_{p})\rho_{p}\sum \eta_{j}R_{j,s}\left[-\Delta H_{rxn,j}(P_{i,s})\right] - a_{v}h_{gp}(z)\left[T_{s}(z) - T(z)\right] \quad \forall z \in (0,L)$$
(23)



• 1D heterogeneous model (M3) = (M1) + interfacial gradients





Reactor Length (m)

Reactor Length (m)

• 1D heterogeneous model (M3) = (M1) + interfacial gradients

Reactor Length (m)



- 1D heterogeneous model (M4) = (M1) + interfacial gradients + intraparticle gradients
- Bulk gas material and energy balances:

$$\varepsilon_b \frac{\partial C_i(z)}{\partial t} + \frac{\partial [C_i(z)U_z(z)]}{\partial z} = a_v k_{i,gp}(z) \left[C_{i,p}(z,r_p) - C_i(z) \right] \quad \forall z \in (0,L)$$
(29)

$$\varepsilon_b \rho_g(z) C_{p,g}(z) \frac{\partial T(z)}{\partial t} + \rho_g(z) C_{p,g}(z) U_z(z) \frac{\partial T(z)}{\partial z} = \frac{4U(z)}{d_t} [T_w(z) - T(z)] + a_v h_{gp}(z) [T_p(z, r_p) - T(z)] \quad \forall z \in (0, L)$$
(30)

• Catalyst material and energy balances:

$$\varepsilon_{p} = \left[\varepsilon_{p}\rho_{g}(z,\xi)C_{p,g}(z,\xi) + (1-\varepsilon_{p})\rho_{p}C_{p,p}\right]\frac{\partial T_{p}(z,\xi)}{\partial t} = \sum_{j}\left[\varepsilon_{p}\mathcal{D}_{i,\xi}^{e}(z,\xi)\frac{\partial C_{i,p}(z,\xi)}{\partial\xi}C_{p,i}(z,\xi)\right]\frac{\partial T_{p}(z,\xi)}{\partial\xi} + \lambda_{\xi}^{e}(z,\xi)\left[\frac{\partial^{2}T_{p}(z,\xi)}{\partial\xi^{2}} + \frac{2}{\xi}\frac{\partial T_{p}(z,\xi)}{\partial\xi}\right] + (1-\varepsilon_{p})\rho_{p}\sum_{j}R_{j}(z,\xi)[-\Delta H_{rxn,j}(z,\xi)] \quad \forall z \in (0,L) \quad \forall \xi \in (0,r_{p})$$

$$\varepsilon_p \frac{\partial C_{i,p}(z,\xi)}{\partial t} = \varepsilon_p \mathcal{D}_{i,\xi}^e(z,\xi) \left[\frac{\partial^2 C_{i,p}(z,\xi)}{\partial \xi^2} + \frac{2}{\xi} \frac{\partial C_{i,p}(z,\xi)}{\partial \xi} \right]$$
$$[1 - \varepsilon_p) \rho_p \sum R_j(z,\xi) \nu_{ij} \quad \forall z \in (0,L) \quad \forall \xi \in (0,r_p)$$

M1 with different effectiveness factor

vs M4

$$\eta_j = \frac{apparent\ reaction\ rate}{intrinsic\ reaction\ rate} = \frac{3\int_0^{r_p} \xi^2 R_j(\xi)\,d\xi}{r_p^3 R_j(r_p)}$$

Why adding effectiveness factor in pseudohomogeneous models?

In order to compensate for the external diffusion resistance and internal diffusion resistance.





6

6

9

12

9

η=1

n=0.01

η=0.001

---- η=0.1

— M4

12

• 1D heterogeneous model (M4) = (M1) + interfacial gradients + intraparticle gradients



• Reactions occur on the near-surface area due to strong diffusion limitations.



• 2D pseudo-homogeneous model (M5) = (M2) + radial mixing

$$\begin{split} \varepsilon_{b} \frac{\partial C_{i}(z,r)}{\partial t} &+ \frac{\partial [C_{i}(z,r)U_{z}(z,r)]}{\partial z} = \varepsilon_{b} \mathcal{D}_{i,z}^{e}(z,r) \frac{\partial^{2}C_{i}(z,r)}{\partial z^{2}} \\ &+ \varepsilon_{b} \mathcal{D}_{i,r}^{e}(z,r) \left[\frac{\partial^{2}C_{i}(z,r)}{\partial r^{2}} + \frac{1}{r} \frac{\partial C_{i}(z,r)}{\partial r} \right] \\ &+ (1-\varepsilon_{b})\rho_{p} \sum \eta_{j}R_{j}(z,r)\nu_{ij} \quad \forall z \in (0,L) \quad \forall r \in (0,r_{t}) \\ &\left[(1-\varepsilon_{b})\rho_{p}C_{p,p} + \varepsilon_{b}\rho_{g}(z,r)C_{p,g}(z,r) \right] \frac{\partial T(z,r)}{\partial t} + \rho_{g}(z,r)C_{p,g}(z,r)U_{z}(z,r) \frac{\partial T(z,r)}{\partial z} \\ &= \lambda_{z}^{e}(z,r) \frac{\partial^{2}T(z,r)}{\partial z^{2}} + \lambda_{r}^{e}(z,r) \left[\frac{\partial^{2}T(z,r)}{\partial r^{2}} + \frac{1}{r} \frac{\partial T(z,r)}{\partial r} \right] \\ &+ \sum \left[\varepsilon_{b} \mathcal{D}_{i,z}^{e}(z,r) \frac{\partial C_{i}(z,r)}{\partial z} C_{p,i}(z,r) \right] \frac{\partial T(z,r)}{\partial z} \\ &+ \sum \left[\varepsilon_{b} \mathcal{D}_{i,r}^{e}(z,r) \frac{\partial C_{i}(z,r)}{\partial r} C_{p,i}(z,r) \right] \frac{\partial T(z,r)}{\partial r} \\ &+ \sum \left[\varepsilon_{b} \mathcal{D}_{i,r}^{e}(z,r) \frac{\partial C_{i}(z,r)}{\partial r} C_{p,i}(z,r) \right] \frac{\partial T(z,r)}{\partial r} \\ &+ \sum \left[\varepsilon_{b} \mathcal{D}_{i,r}^{e}(z,r) \frac{\partial C_{i}(z,r)}{\partial r} C_{p,i}(z,r) \right] \frac{\partial T(z,r)}{\partial r} \\ &+ (1-\varepsilon_{b})\rho_{p} \sum \eta_{j}R_{j}(z,r)[-\Delta H_{rxn,j}(z,r)] \quad \forall z \in (0,L) \quad \forall r \in (0,r_{t}) \quad (43) \end{aligned}$$

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• 2D pseudo-homogeneous model (M5) = (M2) + radial mixing

• 2D pseudo-homogeneous model (M5) = (M2) + radial mixing



- 2D pseudo-homogeneous model (M5)
- Reactions occur in the near-wall areas.
- Process intensification: Energy supplied from inside of the catalyst particles.





• 2D heterogeneous model (M6)

For the reactor domain:

$$\varepsilon_{b} \frac{\partial C_{i}(z,r)}{\partial t} + \frac{\partial [C_{i}(z,r)U_{z}(z,r)]}{\partial z} = \varepsilon_{b} \mathcal{D}_{i,z}^{e}(z,r) \frac{\partial^{2} C_{i}(z,r)}{\partial z^{2}} + \varepsilon_{b} \mathcal{D}_{i,r}^{e}(z,r) \left[\frac{\partial^{2} C_{i}(z,r)}{\partial r^{2}} + \frac{1}{r} \frac{\partial C_{i}(z,r)}{\partial r} \right] + a_{v} k_{i,gp}(z,r) \left[C_{i,p}(z,r,r_{p}) - C_{i}(z,r) \right] \quad \forall z \in (0,L) \quad \forall r \in (0,r_{t})$$
(62)

$$\varepsilon_{b}\rho_{g}(z,r)C_{p,g}(z,r)\frac{\partial T(z,r)}{\partial t} + \rho_{g}(z,r)C_{p,g}(z,r)U_{z}(z,r)\frac{\partial T(z,r)}{\partial z} = \lambda_{z}^{e}(z,r)\frac{\partial^{2}T(z,r)}{\partial z^{2}} + \lambda_{r}^{e}(z,r)\left[\frac{\partial^{2}T(z,r)}{\partial r^{2}} + \frac{1}{r}\frac{\partial T(z,r)}{\partial r}\right] + \sum \left[\varepsilon_{b}\mathcal{D}_{i,z}^{e}(z,r)\frac{\partial C_{i}(z,r)}{\partial z}C_{p,i}(z,r)\right]\frac{\partial T(z,r)}{\partial z} + \sum \left[\varepsilon_{b}\mathcal{D}_{i,r}^{e}(z,r)\frac{\partial C_{i}(z,r)}{\partial r}C_{p,i}(z,r)\right]\frac{\partial T(z,r)}{\partial r} + a_{v}h_{gp}(z,r)\left[T_{p}(z,r,r_{p}) - T(z,r)\right] \quad \forall z \in (0,L) \quad \forall r \in (0,r_{t})$$
(63)



• 2D heterogeneous model (M6)

For the catalyst domain:

$$\varepsilon_p \frac{\partial C_{i,p}(z,r,\xi)}{\partial t} = \varepsilon_p \mathcal{D}_{i,\xi}^e(z,r,\xi) \left[\frac{\partial^2 C_{i,p}(z,r,\xi)}{\partial \xi^2} + \frac{2}{\xi} \frac{\partial C_{i,p}(z,r,\xi)}{\partial \xi} \right] + (1-\varepsilon_p)\rho_p \sum R_j(z,r,\xi)\nu_{ij} \quad \forall z \in (0,L) \quad \forall r \in (0,r_t) \quad \forall \xi \in (0,r_p) \quad (64)$$

$$\begin{split} &[\varepsilon_p \rho_g(z,r,\xi) C_{p,g}(z,r,\xi) + (1-\varepsilon_p) \rho_p C_{p,p}] \frac{\partial T_p(z,r,\xi)}{\partial t} = \\ &\sum \left[\varepsilon_p \mathcal{D}^e_{i,\xi}(z,r,\xi) \frac{\partial C_{i,p}(z,r,\xi)}{\partial \xi} C_{p,i}(z,r,\xi) \right] \frac{\partial T_p(z,r,\xi)}{\partial \xi} \\ &+ \lambda^e_{\xi}(z,r,\xi) \left[\frac{\partial^2 T_p(z,r,\xi)}{\partial \xi^2} + \frac{2}{\xi} \frac{\partial T_p(z,r,\xi)}{\partial \xi} \right] \\ &+ (1-\varepsilon_p) \rho_p \sum R_j(z,r,\xi) [-\Delta H_{rxn,j}(z,r,\xi)] \\ &\quad \forall z \in (0,L) \quad \forall r \in (0,r_t) \quad \forall \xi \in (0,r_p) \end{split}$$



(65)

• 2D heterogeneous model (M6)



2D heterogeneous model (M6) •



• 2D heterogeneous model (M6)





10

12

8

6

Reactor Length (m)

CO Composition

0.050

-0.050

0

0.5226

2

4





Electrification of SMR (In progress)



- Induction heating is generated by an alternating magnetic field, and provides a non-contact heat source.
- Mechanisms: eddy currents, magnetic hysteresis, and magnetic resonance.



Catalyst: providing hysteresis heating. Effective induction heating requires the susceptor to be ferromagnetic.

Curie temperature: the temperature above which certain magnetic materials undergo a transition from being ferromagnetic to paramagnetic.

Ni: Tc = 358 °C Fe: Tc = 770 °C Co: Tc = 1121 °C











Julius Robert Oppenheimer (1904-1967) The Manhattan Project Father of the Atomic Bomb





World First A-bomb: July. 16, 1945 Trinity Test: New Mexico, US.





The atomic bombing of Hiroshima, Japan (in Japanese: 広島市への原子爆弾投下) August 6, 1945





The first atomic bomb test by the Soviet Union occurred on August 29, 1949. This test, codenamed "RDS-1" and also known as "First Lightning," took place at the Semipalatinsk Test Site in the Kazakh Soviet Socialist Republic. This successful detonation marked the Soviet Union as the second nation in the world to possess nuclear weapons, following the United States.



Nikita Khrushchev and John F. Kennedy





Nikita Khrushchev and Mao Zedong







October 16, 1964. Chinese first A-bomb



Who built the Chinese atomic bomb?









Dr. Chia Hsien Teng (邓稼先博士) Father of the Chinese A-Bomb

PhD in Physics, Purdue University, 1950



U N I V E R S I T Ya





Dr. | Sheng Mao (茅以升博士)

First Ph.D. ever granted by the Carnegie Institute of Technology (now <u>Carnegie Mellon University</u>), 1919.



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Dr. Thomson Eason Mao 来以异学唐臣 (Mao I-eheng)



President of National Chiao Tung University





Prof. K.T. Yu (余国琮博士) Ph.D. Univ. Pittsburgh, 1947





Father of Chinese Modern Distillation

Some Facts



In 1958, China's first nuclear reactor became operational. The reactor required heavy water as a moderator, but at that time, China had not yet mastered the technology for producing heavy water independently and mainly imported it from the Soviet Union. After the deterioration of Sino-Soviet relations, China's nuclear energy program faced the threat of coming to a halt. Consequently, overcoming the challenges of heavy water separation and mastering the independent production technology of heavy water became an urgent priority. Ultimately, this significant responsibility fell on the shoulders of Dr. Yu.

Prof. K.T. Yu (余国琮博士) Ph.D. Univ. Pittsburgh, 1947



Heavy water (deuterium oxide, ²H₂O, D₂O) is a form of water whose hydrogen atoms are all deuterium (²H or D, also known as *heavy hydrogen*) rather than the common hydrogen–1 isotope (¹H or H, also called *protium*) that makes up most of the hydrogen in normal water.^[3] The presence of the heavier hydrogen isotope gives the water different nuclear properties, and the increase in mass gives it slightly different physical and chemical properties when compared to normal water.

Some Facts

Deuterium is a heavy hydrogen isotope. Heavy water contains deuterium atoms and is used in nuclear reactors. Semiheavy water (HDO) is more common than pure heavy water, while heavy–oxygen water is denser but lacks unique properties. Tritiated water is radioactive due to tritium content.

Heavy water (D₂O) has different physical properties than regular water, such as being 10.6% denser and having a higher melting point. Heavy water is less dissociated at a given temperature, and it does not have the blue color of regular water. While it has no significant taste difference, it can taste slightly sweet. Heavy water affects biological systems by altering enzymes, hydrogen bonds, and cell division in eukaryotes. It can be lethal to multicellular organisms at concentrations over 50%. However, some prokaryotes like bacteria can survive in a heavy hydrogen environment. Heavy water can be toxic to humans, but a large amount would be needed for poisoning to occur.

Deuterated water (HDO) occurs naturally in normal water and can be separated through distillation, electrolysis, or chemical exchange processes. The most cost–effective process for producing heavy water is the Girdler sulfide process. Heavy water is used in various industries and is sold in different grades of purity. Some of its applications include nuclear magnetic resonance, infrared spectroscopy, neutron moderation, neutrino detection, metabolic rate testing, neutron capture therapy, and the

Heavy water Names **IUPAC** name (²H₂)Water^[4] Other names Deuterium oxide^[1] Water $-d_2^{[2]}$ Dideuterium monoxide Deuterated water^[3] Identifiers CAS Number 7789-20-0 🗗 🗸 3D model (JSmol) Interactive image 🗷 CHEBI:41981 🖉 🗸 ChEBI ChEMBL1232306 27 🗸 ChEMBL ChemSpider 23004 🖉 🗸

100.029.226 🗗 🖉

ECHA InfoCard





Prof. Xingang Li (李鑫钢博士) Ph.D. Tianjin Univ, 1992















Cui et al. Process synthesis and simulation-based optimization of ethylbenzene/styrene separation using double-effect heat integration and self-heat recuperation technology. Sep. Purif. Technol. 2019; 228, 115760





Cui et al. Process synthesis and simulation-based optimization of ethylbenzene/styrene separation using double-effect heat integration and self-heat recuperation technology. Sep. Purif. Technol. 2019; 228, 115760



Electrification of Binary Distillation

U N I V E R S I T Ya



Cui et al. Process synthesis and simulation-based optimization of ethylbenzene/styrene separation using double-effect heat integration and self-heat recuperation technology. Sep. Purif. Technol. 2019; 228, 115760

Electrification of Pressure-Swing Distillation: Design



Electrification of Pressure-Swing Distillation: Design





Cui et al. Electrical-driven self-heat recuperative pressure-swing azeotropic distillation to minimize process cost and CO2 emission: Process electrification and simultaneous optimization. Energy. 2020, 195, 116998.

Electrification of Pressure-Swing Distillation: Design





Cui et al. Electrical-driven self-heat recuperative pressure-swing azeotropic distillation to minimize process cost and CO2 emission: Process electrification and simultaneous optimization. Energy. 2020, 195, 116998.

Table 7-4 Comparison of four process configurations for THT7 water separation								
Item	PSD-CONV	PSD-DED	PSD-HPAD	PSD-SHRT				
Cooling water duty (kW)	3034	2016	588	0				
LPS steam duty (kW)	2499	1360	459	26				
MPS steam duty (kW)	1323	1404	408	253				
Total steam duty (kW)	3822	2764	867	279				
Electrical power (kW)	0	0	637	650				
OPEX (10 ⁶ US\$/a)	0.9040	0.6576	0.5136	0.3801				
Total CAPEX (10 ⁶ US\$)	1.2746	1.2909	3.4804	3.6071				
Annual CAPEX (106US\$/a)	0.1497	0.1516	0.4086	0.4237				
TAC (10 ⁶ US\$/a)	1.0537	0.8092	0.9224	0.8038				
OPEX/TAC ratio	0.8579	0.8127	0.5568	0.4729				
TAC reduction	_	23.20%	12.46%	23.72%				
CO2 emission (kg CO2/h)	1356.7	989.5	427.0	221.5				
CO ₂ emission reduction	_	27.07%	68.53%	83.67%				

 Table 7-4 Comparison of four process configurations for THF/water separation



Cui et al. Electrical-driven self-heat recuperative pressure-swing azeotropic distillation to minimize process cost and CO2 emission: Process electrification and simultaneous optimization. Energy. 2020, 195, 116998.



Control loops:

- 1. Total feed is flow controlled and used as a throughput manipulator.
- 2. Top pressures of each column are controlled by manipulating condenser duties.
- 3. Reflux drum levels are controlled by manipulating distillate flow rates.
- 4. Base levels are controlled by manipulating bottoms flow rates.
- 5. Single-end temperature control in each column.









Key control loops

- 1. Temperature control loops: The temperature is controlled by manipulating W1/F feedforward controller.
- 2. A R1/F feedforward controller is added to stabilize the column.









Extractive distillation: Solvent (or entrainer) usually has much higher boiling point than A/B components to be separated. So using heat pump might not have a high COP.



Cui et al. Process synthesis and simultaneous optimization of extractive distillation system integrated with organic Rankine cycle and economizer for waste heat recovery. J. Taiwan Inst. Chem. Eng. 2019, 102, 61-72.





Cui et al. Process synthesis and simultaneous optimization of extractive distillation system integrated with organic Rankine cycle and economizer for waste heat recovery. J. Taiwan Inst. Chem. Eng. 2019, 102, 61-72.

Table 10-3 Optimization results of the basic ED-ORC system with working fluid selection									
Working	Fwf	Pevap	Pcond	Qin	Wturb	Wpump	Wnet	η	ED-ORC TAC
fluid type	(kmol/hr)	(bar)	(bar)	(kW)	(kW)	(kW)	(kW)		(10 ⁶ US\$/a)
R218	423.52	26.00	13.08	1989.13	181.56	29.30	152.26	7.65%	0.8807
R227EA	317.06	17.20	7.05	1990.07	178.18	14.39	163.79	8.23%	0.8912
RC318	286.05	12.12	4.93	1982.94	161.98	9.97	152.01	7.67%	0.8959
R236FA	273.55	10.99	4.35	1971.60	158.28	7.34	150.94	7.66%	0.8970
R600A	330.43	11.95	5.31	1983.47	166.79	8.33	158.46	7.99%	0.8939
R236EA	265.46	8.46	3.37	1982.54	151.99	5.20	146.79	7.40%	0.8974
R600	301.28	9.01	3.79	1982.63	162.19	5.71	156.48	7.89%	0.8962
R245FA	245.56	7.01	2.52	1997.14	156.46	3.96	152.50	7.64%	0.8997
R245CA	234.79	4.71	1.73	1991.39	145.49	2.41	143.08	7.18%	0.9010
R601A	252.55	3.84	1.51	1983.15	146.36	2.45	143.91	7.26%	0.8999
R601	240.35	3.03	1.16	1982.73	142.95	1.85	141.10	7.12%	0.9008

Extractive distillation-ORC: R227EA has the highest thermal efficiency, and we will use it in process design.





ED-ORC: Save ~30% TAC compared to conventional ED.







Cui et al. Process synthesis and plantwide control of intensified extractive distillation with preconcentration for separating the minimum-boiling azeotropes: A case study of acetonitrile dehydration. Sep. Purif. Technol. 2022, 285, 120397.

Energy consumption and economic cost comparison of different extractive distillation processes.

Process	#1	#2	#3	#4	#4*	#5
Cooling water [kW]	4079	2736	2189	2250	2166	1463
Low-pressure steam [kW]	3456	2011	1343	920	888	0
Medium- pressure steam [kW]	781	740	0	0	0	0
High-pressure steam [kW]	0	0	911	1263	1292	1263
Total hot utility [kW]	4237	2751	2254	2183	2180	1263
Electrical power [kW]	0	88	61	180	84	330
Energy cost [10 ⁶ US\$/a]	1.0008	0.6962	0.6120	0.6755	0.6293	0.5340
Energy cost reduction	0 %	30.43 %	38.85 %	32.50 %	37.12 %	46.65 %
TAC [10 ⁶ US \$/a]	1.3925	1.1071	0.9808	1.1375	1.0162	1.1039
TAC reduction	0 %	20.49 %	29.57 %	18.32 %	27.03 %	20.72 %



Cui et al. Process synthesis and plantwide control of intensified extractive distillation with preconcentration for separating the minimum-boiling azeotropes: A case study of acetonitrile dehydration. Sep. Purif. Technol. 2022, 285, 120397.

Electrification of Extractive Distillation: Control





Cui et al. Process synthesis and plantwide control of intensified extractive distillation with preconcentration for separating the minimum-boiling azeotropes: A case study of acetonitrile dehydration. Sep. Purif. Technol. 2022, 285, 120397.



- 1. **Decarbonization**: Electrification of catalytic reactor and distillation can achieve lowcarbon production if renewable energy is used.
- 2. Process intensification: Electrified catalytic reactor and distillation processes can generally save energy consumption and reduce TAC. They have steady-state economic advantages.
- 3. **Process control**: Electrified distillation processes have general good control performances that could be compete with conventional distillation processes.

