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Chemicals – Energy – Water (CEW) Nexus for Sustainable Process Design

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Rising demand for greener technologies, increasing competition, growing utility complexities, and evolving resource and environmental issues are some of the important factors reshaping chemical industry. For this, Chemicals, energy and water (CEW) nexus concept is introduced. This nexus is a complex interaction, and the production and supply of any resource affects the other two resources. A generalized CEW nexus model is proposed for process design. A cooling water system is illustrated as a case study. We investigated integrated collaborative management policies on CEW nexus. These contribute to the trend of accelerating the decarbonization of industrial production.

1. Introduction

Sustainable management of chemicals, energy, and water is an important part of the UN Sustainable Development Goals (SDGs), which require humans to operate in an integrated manner (Simpson et al., 2016). The chemical industry serves as the carrier of chemicals, energy, and water, all of which are closely interrelated. The energy-water nexus exists as water is involved in the energy production, while water supply and wastewater treatment need to consume large amounts of energy (Kirchem et al., 2020). Similarly, chemicals-water nexus characterises the transformation of these chemicals during chemical reactions. Chemicals-energy-water (CEW) nexus offers a holistic approach to quantify these interrelationships, as shown in Figure 1. The nexus perspective is considered as an effective approach for pursuing sustainable development. The quantification of these relationships is the first step towards incorporating relational models that contribute to sustainable production and consumption (Peña-Torres. et al. 2024.)
While numerous existing studies on energy-water nexus have managed to optimize the energy and water network, the chemicals have often been a neglected element of analysis. To this end, this study takes circulating cooling water system as an example and quantitatively depicts the relationships among chemicals, energy and water. This study can provide suggestions both for saving resources and reducing carbon emissions based on sustainable development policies for chemical industry and beyond.

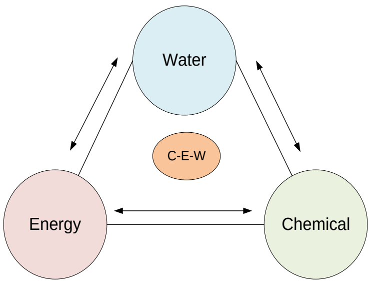

Figure 1: Conceptual diagram of CEW nexus

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2. Methodology

2.1 Determination of system boundaries

The circulating cooling water system is classified according to chemicals, energy and water. The module division and material flow relationship between the systems are shown in Figure 2. The system boundary is determined according to the material exchange process of the circulating cooling water tower, including the cooling tower, water pump, heat exchanger, and side filter pump.

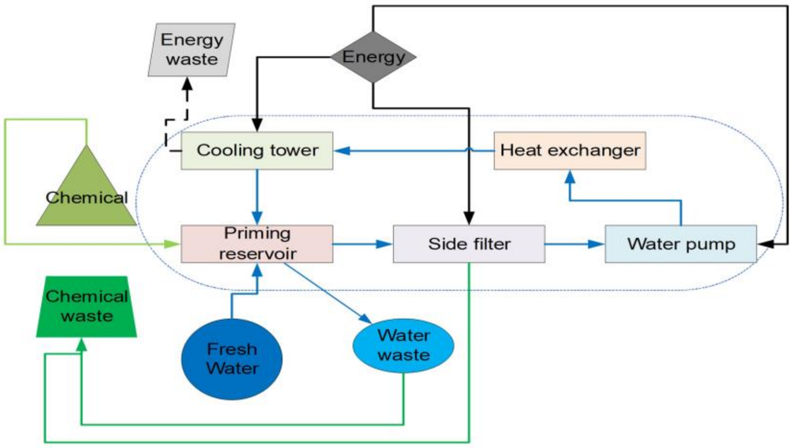

Figure 2: Flow diagram of circulating cooling water system

2.2 Mathematical model

(1) System boundary

The system is divided into five modules, i.e., cooling tower, suction ponds, the side filter, water pumps and heat exchangers.

(2) Water network

The flowrate balance of water in the sub-modules is shown as Eq(1).

$$W_{out} = Q_x W_{in} \tag{1}$$

Water flow components is shown as Eq(2).

$$W_w = \{W_{x_1}, W_{x_2}, W_{x_3} \dots W_{x_x}\} \tag{2}$$

Qx is flow composition coefficient matrix x stands for a reaction module in a chemical reaction; W_{out} means outlet water flow, W_{in} means Inlet water flow. W_w means the composition of the water flow rate of all sub-modules within the system, and is the set of all water flows.

$$\sum_j f_j + \sum_{k \neq j} f_{k,j} = \sum_j W_j + \sum_{j \neq k} f_{j,k} \tag{3}$$

f_j represents the inlet water flow rate. $f_{k,j}$ represents the amount of water used from k to j. W_j represents the amount of water exported. $f_{j,k}$ the flow of water from j to k. This process does not include the addition of chemicals.

(3) Energy network

The energy balance of energy in the sub-modules is shown as below:

$$E_{out} = Q_x E_{in} \tag{4}$$

$$E_w = \{E_{x_1}, E_{x_2}, E_{x_3} \dots E_{x_x}\} \tag{5}$$

E_{out} means outlet energy flow, E_{in} means Inlet energy flow. E_w means the composition of the energy flow rate of all sub-modules within the system, and is the set of all energy flows.

(4) Network distribution of chemicals

Electrical conductivity of the added agent:

$$\sigma = \sum_{i=1} \left[C \left(1000M \sum_{i=1} \mu \right) / Q \right] \tag{6}$$

$$N = \frac{\mu_C}{\mu_M} \tag{7}$$

The increase in conductivity with the addition of chemicals to the circulating cooling water is a combination of concentration, molecular weight, resulting ionic conductivity and solvent volume. This will be of vital help in the subsequent study of the C-E-W network. The specific mathematical model for CEW composition flow embodiment, as shown in Eqs (2-4).

3.Case study

To quantitatively depicts the relationships among chemicals, energy and water, this study assumes a circulating water flow rate of 4000 t/h and selects a mechanical ventilation cooling tower (Wang et al., 2023), as shown in Figure 3.

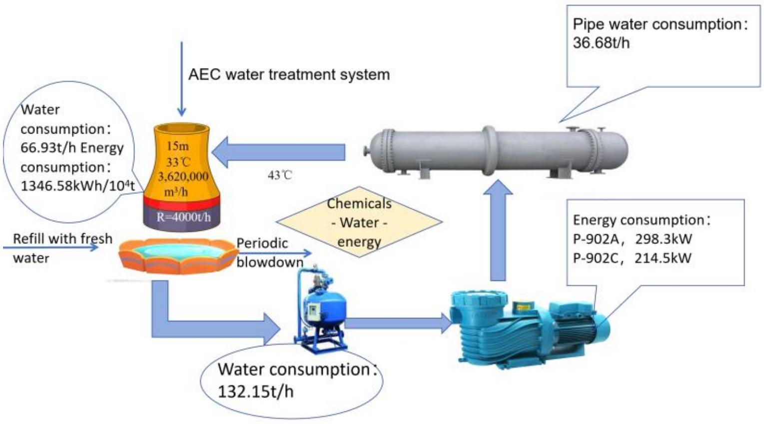

Figure 3: Circulating cooling water system diagram

3.1 Water consumption

Cooling tower consumption involves evaporation and splashing in the cooling tower, Water loss from periodic discharge, and Fresh water supplement.

A: Water loss by evaporation (E)

In the cooling tower, the amount of water lost by evaporation of the cooling water is related to the climate and cooling amplitude, and is usually expressed by the evaporation loss rate. The more water that goes into the cooling tower, the more E is lost, α is rates of evaporative loss, specific water evaporation losses are as follows.

$$E = \alpha(R - B) = 37.76\,\text{t/h}$$
$$\alpha = \mathrm{e}(t_1 - t_2)\% \tag{8}$$

B: Splash loss (wind loss) (C)

The amount of splash loss of cooling tower depends on the design type of cooling tower, wind speed and other factors. Under normal circumstances, its value is equal to about 0.1%~0.2% of the circulating water. In this case, the splash loss is 4 t/h.

C: Water loss from periodic discharge (B)

The loss of normal discharge water depends on factors such as water quality or solids concentration in the water. It is generally about 0.3% of the circulating water, which is shown in Eq(9).

$$B = E / (k - 1) \approx 25.17\,\text{t/h} \tag{9}$$

M: Fresh water supplement

When the pipes in the system are connected tightly and no leakage occurs, F=0; M Replenishment equals the sum of E (Evaporation losses), W (Wind losses), B (Sewage discharge), and F. The final fresh water replenishment produced is M=37.76 t/h+4 t/h+25.17 t/h +0=66.93 t/h. Water consumption of bypass filter can be seen in Eq(10).

$$Q_{sf} = [Q_m C_{ms} + K_s C_a \mathrm{A} - (Q_b + Q_w)\mathrm{Cr_s} + QC_z]/(Cr_s - C_{ss}) = 3484.3\,\mathrm{t/h} \tag{10}$$

3.2 Energy consumption

The energy consumption in the whole process mainly includes: pump energy consumption, and cooling tower energy consumption. The energy required by the water pressure includes the head loss of the whole pipeline and the pressure relief of the local equipment valve. The distance difference energy consumption refers to the energy consumed to overcome the long-distance water supply. Integration through heat pumps will reduce energy consumption (Klemeš et al., 2016). Pump selection can be seen in Figure 3.
The main pump is P-902A, and its calculation formula is shown as Eq(11).

$$W = \frac{\rho g\, qH}{1000\,\eta_1\eta_2} t = \frac{980 q_v \left(0.04 q_v^2 - 2.29 q_v + 44.21\right)}{0.52 q_v^2 - 7.23 q_v + 101.2} = 298.3\mathrm{kW} \tag{11}$$

Power consumption of fan in cooling tower is shown as Eq(12).

$$P_{p,i} = \frac{2.87\,\mathrm{q_i}\, H}{1028\,\eta_\mathrm{p}} = 1346.58\,\mathrm{kWh}/10^4\,\mathrm{t} \tag{12}$$

3.3 Chemicals consumption

Specifically in the circulating water turbidity treatment before the natural precipitation of raw water, adding flocculants for coagulation, coagulation and then precipitation, and finally get to meet the requirements of the circulating cooling water, the above steps cycle twice a week. The dosing system selected for this article is the AEC water treatment system, which has three components. Details for water data can be found in Table 1.
100-120 mg/L AEC3119 scale and corrosion inhibitor dispersant and 20 mg/L POT6101 high efficiency corrosion inhibitor was dosed with chlorine dioxide at a flow rate of 20 kg/h, and alginate biocide was dosed for about 6 h at a time, supplemented by regular (weekly) shock dosing of non-oxidizing biocide NX1100 and BD1501.

Table 1: Average data of circulating water quality

Variables		Circulating water	Make-up water
Electric conductivity	μ s/cm	4758	865
Total hardness	(mg/L $CaCO_3$)	810	230
Calcium hardness	(mg/L $CaCO_3$)	370	100
Total alkalinity	(mg/L $CaCO_3$)	280	100
Total iron	(mg/L)	0.27	0.04
Chlorogenic	(mg/L)	390	120
Turbidity	(NTU)	15	5
pH		8.42	8.38

4.CEW nexus

4.1 Pairwise nexus

(1) Chemical-Water nexus
Corrosion inhibitor, scale inhibitor and bactericide are regularly added to the suction ponds, the conductivity of circulating water is maintained as 4758 μs/cm, N=5.5, and the discharge volume B≈ E/(K-1) ≈4.02 t/h. It is determined that 66.93 t/h needs to be added fresh water. After replenishing fresh water, circulating cooling water flows into the cooling tower for cooling through the side filter pump, pump and heat exchanger. The circulation reflects the quantitative relationship between chemical substances and water. Changes in water quality will inevitably affect the circulating water flow rate, and variations in water quantity will impact energy consumption.
(2) Energy-Water nexus
As the concentration ratio of circulating water increases, the quality of circulating water changes, with conductivity reaching 4758 μs/cm. The density of the circulating water also changes. Before the pump starts, both the pump and the inlet pipe are filled with water. When the water pump is running, the centrifugal force generated by the high-speed rotation of the impeller throws the water in the impeller channel outward and compresses it into the volute. A vacuum forms at the impeller inlet, causing pool water to be drawn in through the suction pipe due to external atmospheric pressure, thereby replenishing this space. The inhaled water is then expelled by the impeller and flows into the outlet pipe through the volute. The centrifugal force generated by the high-speed rotation of the impeller is closely related to the density of the liquid, and the variations in density also affect the pump head and piping losses. Thus, the energy consumption of the pumping process

varies with water quality, and the overall pump pressure loss (H_t) is the sum of head loss and pipe loss pressure in the group.
The entire pump power is shown in Eq(13).

$$P_t = QH_t \tag{13}$$

It can be seen that the power of the pump is related to both static and dynamic pressure, and the total resistance in the entire water system, that is, the pump head. That is Eq(14)shows:

$$H = \Delta h + \sum_{n=1}^{n} i_n + \frac{u^2}{2g} \tag{14}$$

Velocity head≈0，the specific energy consumption formula of the pump is Eq(11).
It is also possible from the modeling of the pump energy consumption rate, as Eq(15).

$$\frac{\partial}{\partial t}\left(\varepsilon\overline{\Phi}_f\right)+\frac{\partial}{\partial x_k}\left(\varepsilon\overline{\Phi}_f\overline{V}_{fk}\right)=\frac{\partial}{\partial x_k}\left[\overline{\Phi}_f\left(v_f+\frac{v_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_k}\right]+\left[C_{\varepsilon 1}P_r-\overline{\Phi}_f\left(C_{\varepsilon 2}\varepsilon+C_{\varepsilon 3}A_{DS}\right)\right]\frac{\varepsilon}{K} \tag{15}$$

It is closely related to the particle concentration and size in the fluid and the slip amount between the particle and the fluid, as shown in Eq(16).

$$Q = W_2 C_{p2}\left(t_2 - t_1\right) = \mathrm{KA}\,\Delta t_m$$

$$\frac{1}{K} = \frac{1}{\alpha} + R_1 + \frac{\delta}{\lambda}\frac{d_1}{d_m} + R_2\frac{d_1}{d_2} + \frac{1}{\alpha_2}\frac{d_1}{d_2} \tag{16}$$

The selected heat exchanger is E-224A tower kettle cooler, and the theoretical value of heat load design is Q=406513 kcal/h; The actual value of heat load is Q=316.42 kcal/h; The average heat transfer coefficient K=450.6 kcal/h·m^2·℃=524.08 W/m^2·℃.
(3) Chemical-Energy nexus
Corrosion inhibitors, scale inhibitors, and bactericides need to be added regularly to the suction pool. After circulating cooling, the conductivity of circulating water reaches 4,758 µs/cm, with N=5.5, a discharge volume of 4.02 t/h, and a fresh water replenishment rate of 66.93 t/h. The circulating water, after passing through the side filter pump, enters the main pump, and the energy consumption of the pump is described by Eq(11). The energy consumption of the pump has a direct relationship with the density of the circulating water. The circulating water then flows from the pump into the heat exchanger for heat exchange with the external environment, as described by Eq(16). The heat load of the heat exchanger affects the final volume of circulating water required. Additionally, variations in the heat exchanger's location result in different pump head and flow rates, which in turn cause differences in the pump's energy consumption. This process reflects the relationship between energy and chemicals.

4.2 Chemical-Energy-Water nexus

Specific flow relationship can be analyzed from the perspective of chemicals to begin with, after adding chemicals, first determine the conductivity of the circulating water is 4758 µs/cm, and then the concentration ratio also becomes N=5.5. After sewage treatment, the amount of fresh water added becomes 66.93 t/h, the density of the circulating water with the change of the water quality changes, in fact, it is the relevant Chemicals-Water. As the working principle of the pump is before the start of the pump, the pump and the water inlet pipe is full of water, after the pump is running, under the action of the centrifugal force generated by the high-speed rotation of the impeller, the water in the pool in the outside world under the action of atmospheric pressure along the suction pipe is sucked in, the sucked-in water is thrown by the impeller, through the vortex channel into the water outlet pipe, which embodies the impact of the relevant Water-Energy.
The centrifugal force generated by high-speed rotation of the impeller is closely related to the density of the liquid, which also causes the energy consumption of the pump treatment process to vary with the water quality, as Eq(11), and then the energy consumption of the pump changes with the density of the circulating water, the turbidity in the circulating water increases, the operation efficiency of the pump is huge, the friction between the filler and the shaft sleeve significantly increases, and the friction between the outer surface of the impeller and the water increases. The rotation of the impeller needs to overcome the friction and resistance of the water, and the mechanical damage increases, so the energy consumption of the pump is closely related to the density of the circulating water. Heat exchanger heat load scaling increases, cooling efficiency is reduced, and more circulating cooling water is required, resulting in changes in the amount of water pumped by the pump, and the position of the heat exchanger determines the size of the pump head, circulating water and pump head jointly determine the previous pump energy consumption, resulting in changes in energy consumption.

As shown in Figure 4, in the circulating cooling water system, accompanied by a variety of material resources consumption and output, 4000 t/h of cooling water from the cooling tower suction pool outflow, after the bypass filtration pump filtration into the pump, the pump from the outside world to obtain the energy will be circulating water pumped into the heat exchanger for heat exchange, the energy to get the output, the chemical substances in the whole process, accompanied by the entire system of the cooling water cycle. Whether from the perspective of chemicals, water or energy, changes in one resource will inevitably lead to changes in the other two resources in the entire nexus, such as changes in water resources will further lead to changes in the energy consumption of sub-modules of the entire system.

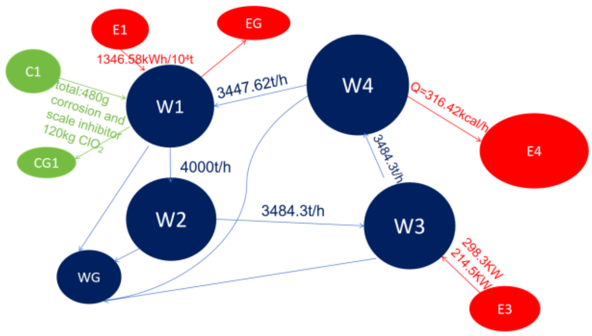

Figure 4: Directed bipartite graph of material flow

5. Conclusions

In a chemical process system, whether from the perspective of chemicals, water, or energy, the production, processing, transportation, storage and consumption of one of the three resources will inevitably lead to the consumption of the output of the other two resources. The quantitative relationships for CEW nexus in process analysis is described. A circulating cooling water system is used as the simulation case to demonstrate the metabolism of chemicals, water, and energy.

Acknowledgments

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