



Novel Conceptual Models for Thermodynamic Analysis of Urban Water Systems

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ABSTRACT

Urban water system (UWS) can be thermodynamically analysed by calculating the entropy budget based on the increase of entropy due to internal and/or external contributions. From different internal and external parts, two novel conceptual models of thermodynamic analysis for an UWS were proposed. For conceptual model 1, natural UWS as a pseudo-reversible process is internal contribution, while the external part of the UWS is artificial water cycle. When the entropy change of the natural UWS is equal to zero, the entropy change of the UWS is considered as the entropy change by the artificial water cycle. The calculations of entropy change for artificial water cycle are based on water balance and purification reactions of selected kinds of typical pollutants in the UWS. For conceptual model 2, the internal entropy change of the UWS is water body, and it is assumed to be zero due to dynamically equilibrium of the water body. The calculation of external entropy change caused by the natural water cycle was proposed to be dependent on meteorological and hydrological data whilst the external entropy change caused by the artificial water cycle could be obtained from mass balance and treatment process analysis.

Keywords: Urban water system; Thermodynamic analysis; Entropy; Conceptual model

1. INTRODUCTION

Urban water system (UWS) is seriously affected by human activities, such as population growth, building, traffic, industries, agriculture, etc. (Sukopp, 1999). Growing population and rapid urbanization have resulted in excess demand and over usage of water, causing the drastic conflicts between water demand and supply towards shortages of water in the city and increasing water pollution (Haase, 2009). This phenomenon is considered as a major driving force in increasing non-point source pollution (Tang et al., 2005) which led to the

incomplete interaction between various flow compartments of the aquifer (Kazemi, 2010), and depredated the groundwater resource (Foster, 2001). Thus, it is necessary to analysis the composition of the UWS, and to find a method for assessing the impact of urban water environment.

Recently, the thermodynamic principles have been widely applied for evaluating of water resources availability, and entropy production of ecosystems has been calculated to investigate the development, growth, and aging of ecosystems (Maruyama et al., 2005; Marchettini et al., 2008). Aoki (1995) found that the entropy production in a lake increases with time during the processes of ecological

succession from oligotrophy to eutrophication. The Min-Max principles indicated that the specific dissipation function and the specific entropy production have two phases of early increase and later decrease with time in aquatic communities (Aoki, 2006, 2008). Besides, the thermodynamic indices were used as ecological indicators of the state of agroecosystems (Steinborn and Svirezhev, 2000) and lake ecosystems (Ludovisi and Poletti, 2003).

The UWS is an open system which exchanges energy (incoming solar radiation and outgoing heat irradiation) and matter (e.g. water, nutrients, organic matter, etc.) with the environment (Jørgensen and Svirezhev, 2004). As it can be considered as an ecosystem, the thermodynamic analysis can be applied to UWS as well as ecosystems. According to previous studies, most of assessments are based on the qualitative analyses for the natural systems by using the entropy indicators. However, they are lack of available models to quantitate an ecological system which is mainly affected artificially. Therefore, as the UWS is dominated by artificial effects on natural water system, the development of quantitative thermodynamic analysis of the UWS is promising.

As such, this study aims to introduce both the basic concepts of thermodynamics and UWS towards establishing a conceptual model of thermodynamic analysis for UWS.

2. THERMODYNAMIC THEORY — ENTROPY

The concept of entropy is important in classical and non-equilibrium thermodynamics. The First Law of Thermodynamics is based on a concept of energy, while the Second Laws of Thermodynamics concern entropy. As a basic thermodynamic property, entropy can characterize all of the ideal and real systems (Serdyukov, 2007).

2.1 Definition of Entropy

Entropy is a macroscopic measure of the microscopic state of disorder or chaos in a system, the higher the entropy, the larger the disorder or chaos inside the system. The laws of thermodynamics indicated that the entropy will either increase or remain the same in any cyclic process. It can also be exchanged with other systems and in particular by exchange of heat. In its most available form, entropy (or entropy change) is revealing the relationship between heat Q and temperature T (Čápek and Sheehan, 2005).

2.2 Calculation of Entropy

According to the Second Law of Thermodynamics, the entropy change (ΔS) of a system can be calculated by the integral (Lukas et al., 2007):

$$\Delta S = S_2 - S_1 = \int_1^2 \frac{dQ_{rev}}{T} \quad (1)$$

where 1, 2 are state 1 and state 2, respectively; dQ_{rev} is the infinitesimal amount of heat transferred to the system undergoing a reversible transformation from state 1 to state 2; T is absolute temperature. Since $dQ_{rev} = C_p dT$ (Gillett, 2006), where C_p is the heat capacity at constant pressure, the entropy change of the system is as follows:

$$\Delta S(T) \geq \int_{T_1}^{T_2} \frac{C_p dT}{T} \quad (2)$$

where, the inequality ($>$) refers to irreversible processes.

For a chemical reaction or process within the system with the standard conditions at 298.15K and 1 bar, the standard entropy change (ΔS^0) can be calculated by Eqs.3 and 4. (Battley, 1999):

$$\Delta S^0 = \frac{\Delta H^0 - \Delta G^0}{T^0} \quad (3)$$

where, ΔH^0 is standard enthalpy of reaction; ΔG^0 is standard Gibbs free energy of reaction; and T^0 is 298.15K.

$$\Delta S^0 = \sum v_{prod} \Delta_f S_{prod}^0 - \sum v_{react} \Delta_f S_{react}^0 \quad (4)$$

where, v_{prod} and v_{react} are the stoichiometric coefficients of each product and reactant, $\Delta_f S^0$ is standard entropy of formation, and the subscripts 'prod' and 'react' represent products and reactants, respectively. Moreover, the thermodynamic data of pure substances can be looked up in the NIST-JANAF thermochemical Tables (Chase, 1998).

3. URBAN WATER SYSTEM (UWS)

As a result of artificial impacts on the natural water system, the UWS is strongly influ-

enced by human activities (Sukopp and Starfinger, 1999). Principally, natural water body can provide necessary fresh water resources for human beings through a series of natural hydrological cycles. However, with the industrialization and urbanization, the human need to build large-scale water supply and drainage facilities. The formation of the large-scale artificial water cycle is then added to the natural water system and thus the UWS is appeared.

Various activities and cycles related to the water can refer to the UWS which is dependent on definitions of the observers. Table 1 shows the different composition of the UWS and Figure 1 (Schütze et al., 2002a) shows the detail subsystems of the UWS.

Table 1 Composition of the UWS

Composition of the UWS	References
Water resources, water demand system, wastewater treatment plant	Lim et al., 2010
Impoundment, water treatment, distribution, collection, sewage treatment and water recycling	Friedrich et al., 2009
Water supply, wastewater disposal, and stormwater runoff systems	Mitchell et al., 2001
The drinking water catchment, the dam, water treatment plant, the community, sewage treatment plant and waterways	Fane, 2005

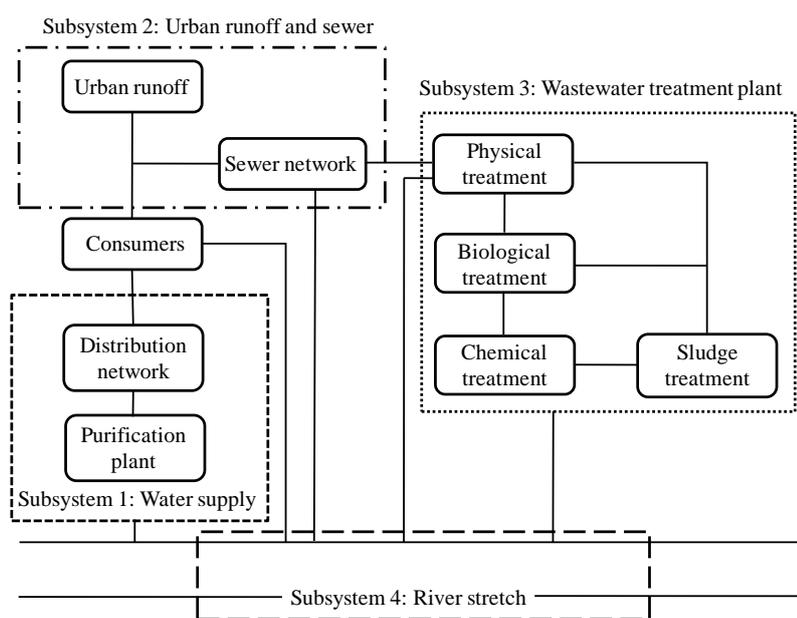


Figure 1 Subsystems of the UWS

If wastewater reuse is considered, there are two kinds of UWS, including linear water system and integrated water cycle system (Lim et al., 2010). Figure 2 illustrates the composition

of the two systems. The difference between two systems is whether the treated wastewater is reused.

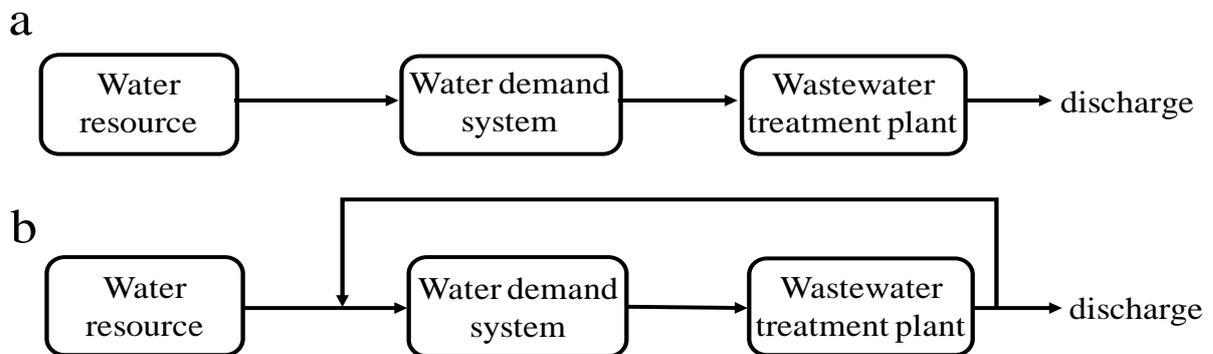


Figure 2 Two kinds of UWS: (a) linear water system; (b) integrated water cycle system

Furthermore, based on the behaviour of water cycle in the urban area, the UWS consists of two water cycles, which are hydrological cycle and artificial water cycle. Thus, the whole UWS can be divided into natural part and artificial part.

3.1 Natural UWS

Natural UWS is composed of water body and the hydrological cycle which natural phenomena occur. Water body includes the water resources such as river, canal, lake, reservoir, dam, stream, transitional water or a stretch of coastal water, groundwater, rainwater and stormwater (Lim et al., 2010, Moglia et al., 2010). Meanwhile, it is also a foundation of hydrological cycle. In a worldwide scale, this cycle contains three main natural processes: evaporation, precipitation, and runoff. Such a water cycle is important for keeping a worldwide or regional circulation of water in various water bodies. Moreover, the water cycle is also a process of water purification that ensures the provision of fresh water resources in the cycle by a series of physical, chemical, and biological reactions (Kundzewicz, 2008).

Overall, the natural UWS is the basis of the artificial UWS.

3.2 Artificial UWS

The configuration of an artificial UWS is considered under the concept of water cycle behaviour. Following the composition discussed above, the basic subsystems for such an artificial UWS are: (i) water supply subsystem; (ii) water use subsystem; (iii) urban drainage subsystem. Apart from these, wastewater reuse subsystem is alternative. According to previous studies, water supply system includes water treatment process and infrastructure, while water use system involves different categories of water use, such as residential, commercial, industrial and agricultural uses (Fagan et al., 2010). The urban drainage (wastewater) system has three components, namely sewer system, wastewater treatment plant and the receiving water body (e.g. river, sea, etc.) (Mannina et al., 2004; Fu et al., 2008, 2009; Freni et al., 2009). The structure of artificial UWS is depicted in Figure 3.

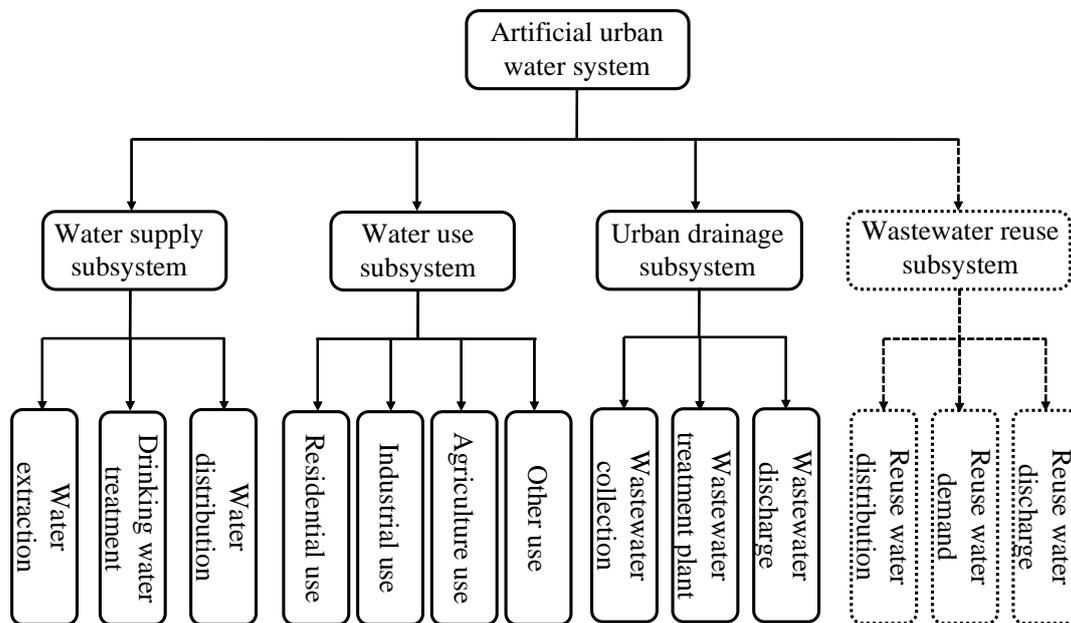


Figure 3 Structure of an artificial UWS (dotted line refer to the system is alternative)

In brief, the UWS is regarded as many artificial water cycles overlaid upon a natural water cycle (hydrological cycle). From a nature-centric point of view, these artificial cycles relate to various human activities for water utilization expose both disturbances on water quantity through water withdrawal and on water quality through pollutant discharge. Therefore, the UWS can be considered as a water ecosystem which the dominant factor is human activities.

4. THERMODYNAMIC ANALYSIS OF AN UWS

According to the thermodynamic theory, for open systems, the total variation of entropy can be expressed as: $dS = d_iS + d_eS$, where entropy production $d_iS = dQ/T$, dQ is the heat production caused by irreversible processes within the system and T is the temperature (K) of the system. The term of entropy flow d_eS corresponds to the entropy of exchange processes between the system and its environment.

Since UWS is an open system, just like an ecological system, thermodynamic analysis is a useful tool to assess it. The change in entropy content for an ecosystem is the sum of two terms: $\Delta S = \Delta_iS + \Delta_eS$, where Δ_eS is an external contribution from outside and Δ_iS is an endogenous contribution due to the internal processes (Ludovisi and Poletti, 2003). The quantities of Δ_eS and Δ_iS are calculated in the ecosystem using of some thermodynamic methods. For example, in the studies of the lake ecosystem which are dominated by natural factors, the Δ_eS was related to the following aspects such as entropy change due to shortwave absorptions, long wave infrared radiation, evaporation, conduction-convection, rain precipitation, water flow outgoing through effluents, water withdrawal and other water losses, and other factors. As for the endogenous contribution, $\Delta_iS = \Delta Q_i/T_w$, where ΔQ_i is the change in heat storage in the lake, and T_w is the mean temperature of lake water (Aoki, 1987, 1995; Ludovisi and Poletti, 2003).

The UWS includes natural water systems and artificial water systems which has many artificial water cycles that overlaid upon a natural water cycle. To set up the methods for quantity of the entropy change of UWS, it is necessary to pick out the internal and external compositions. When evaluating the impact of human activities on the UWS, natural UWS can be seen as the internal composition, and when understanding the evolution of the UWS, natural water cycle can be then considered as the external composition. Thus, two novel conceptual models of thermodynamic analysis for UWS were proposed due to different compositions of internal and external parts.

5. CONCEPTUAL MODELS

5.1 Conceptual Model 1 – Natural Water Cycle Is Internal Part

As mentioned above, all the natural processes in the hydrological cycle is considered as internal processes that bring about endogenous contribution to changes in entropy, while the artificial water cycle can be considered as the external contribution of the entropy change. As a result, the entropy change of UWS (ΔS) is expressed as:

$$\Delta S = \Delta_e S + \Delta_i S \quad (5)$$

where $\Delta_i S$, entropy change caused by natural UWS; $\Delta_e S$, entropy change caused by artificial UWS.

Ecosystems are conceived as self adapting and self-organization systems (Haag and Kaupenjohann, 2001; Jørgensen et al., 1998). They have many properties that are dynamically equilibrium, dynamically stability, self-resilience, self-purification capability, and self-sustaining capability (Suding et al., 2004; Amemiya et al., 2005). Therefore, there are three following assumptions for natural water system:

- (1) Global natural water cycle is an isolated system under a condition of freedom from human disturbance;
- (2) Global natural water cycle can be taken as pseudo-reversible by its nature of self maintenance of water and materials balance in a comparatively short time span (e.g. the time scale of human life) but not a long time span (e.g. the time scale of natural evolution); and
- (3) The natural part of the UWS can be taken as part of the global natural water cycle that also has the above characteristics.

Although any natural process can only progress in a direction which results in an entropy increase (Ludovisi and Poletti, 2003), based on the above assumption, it may be reasonable to infer that the processes of natural UWS would also be a pseudo-reversible. It is well known that the entropy increase of a reversible isolated system is equal to zero by the Second Law of Thermodynamics. Thus, the entropy increase of the natural UWS is inferred to $\Delta_i S \rightarrow 0$, which can be denoted as $\Delta_i S = 0$.

On the basis of Eq.(6), it is necessary to know the calculation of entropy increase $\Delta_e S$ due to artificial water cycle. From the foregoing analysis, the artificial water system has three mainly subsystems: water supply subsystem, water use subsystem and urban drainage subsystem, and one alternative part – wastewater reuse subsystem. These subsystems lead to artificial water cycle. From a nature-centric viewpoint, these artificial water cycles that are related to various human activities for water utilization expose both disturbances on water quantity through water withdrawal and on water quality through pollutant discharge. In this way, a new conceptual model for thermodynamic analysis of an UWS can be depicted in Figure 4.

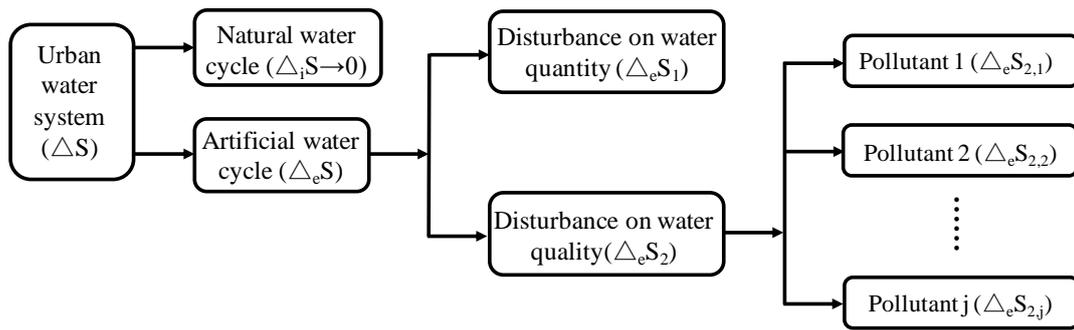


Figure 4 Conceptual model 1 of entropy analysis for an UWS

According to the water balance, the entropy change due to disturbance on water quantitative can be obtained. For the qualitative contribution of entropy, it can be gained from purification reactions for pollutants which were existed in the water environment. J kinds of typical substances were selected and base on the calculation of entropy for reactions, entropy change due to disturbance on water quality can be calculated.

Therefore, the entropy change of UWS is expressed as

$$\Delta S = \Delta_e S = \Delta_e S_1 + \Delta_e S_2 = \Delta_e S_1 + \sum_j \Delta_e S_{2,j} \quad (6)$$

where $\Delta_i S$, entropy change cause by natural water cycle; $\Delta_e S$, entropy change cause by artificial water cycle; $\Delta_e S_1$, entropy change due to disturbance on water quantitative; $\Delta_e S_2$, entropy change due to disturbance on water quality; $\Delta_e S_{2,j}$, entropy change due to j kinds of typical substances.

This kind of conceptual model has already been used to analysis of an urban water system in Xi'an, China (Wang et al., 2011).

5.2 Conceptual Model 2 – Natural Water Cycle Is External Part

When the natural water cycle and the artificial water cycle were considered as external parts, the internal part is the water body. Eq.(6) is also used to calculate the entropy change of the UWS; however, in this case, $\Delta_i S$ is internal

entropy change of the water body, and $\Delta_e S$ is the sum of entropy change of natural water cycle and the artificial water cycle process.

Based on the analysis of UWS, the entropy of natural water cycle process is composed of three major processes (evaporation, precipitation and runoff), and the artificial water cycle is made up by its subsystems of compartments. A conceptual model of thermodynamic analysis for the UWS can be then established. Figure 5 shows the proposed conceptual model for thermodynamic analysis of an UWS which natural water cycle is considered as internal part.

For the entropy change associated with evaporation, precipitation and runoff can be calculated using the meteorological and hydrological data (Aoki, 1987). However, there is no method to calculate the entropy change due to artificial water cycle. Figure 6 shows two cases of artificial water cycle with and without wastewater reuse subsystem. Without wastewater reuse, the water flows through subsystems for water supply, water use and drainage treatment, and then discharges into the water body. With wastewater reuse subsystem, the water flows through subsystems of water supply, water use and urban drainage, and goes into wastewater system afterwards rather than discharges into the water body, and then the reuse water can be used by water supply subsystem.

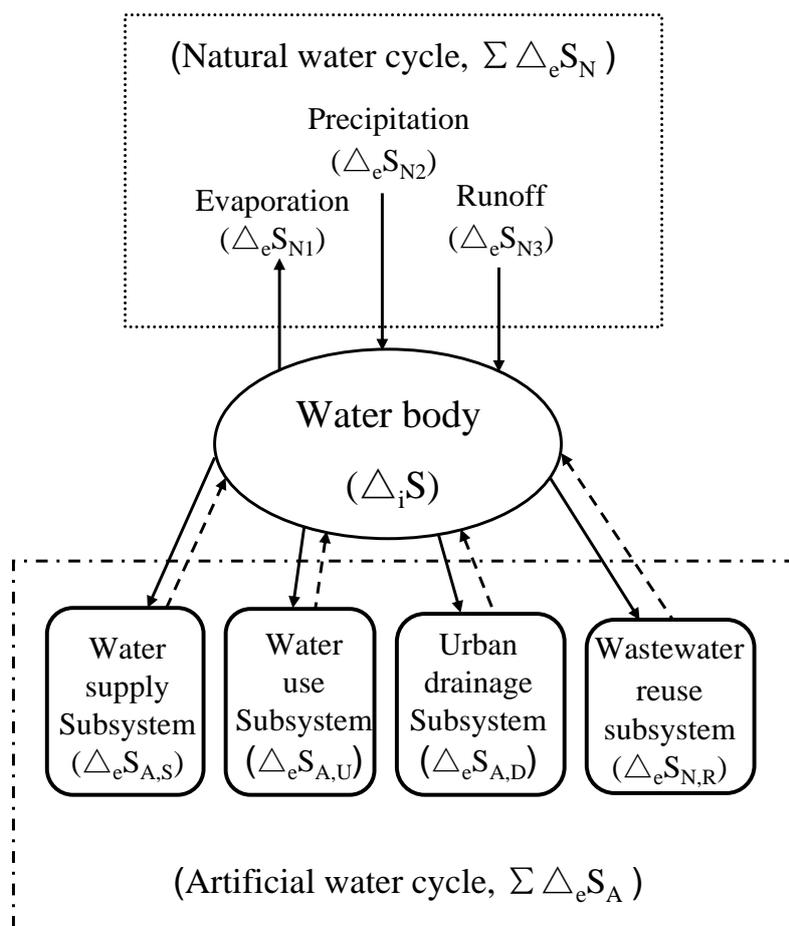


Figure 5 Conceptual model 2 of thermodynamic analysis for an UWS

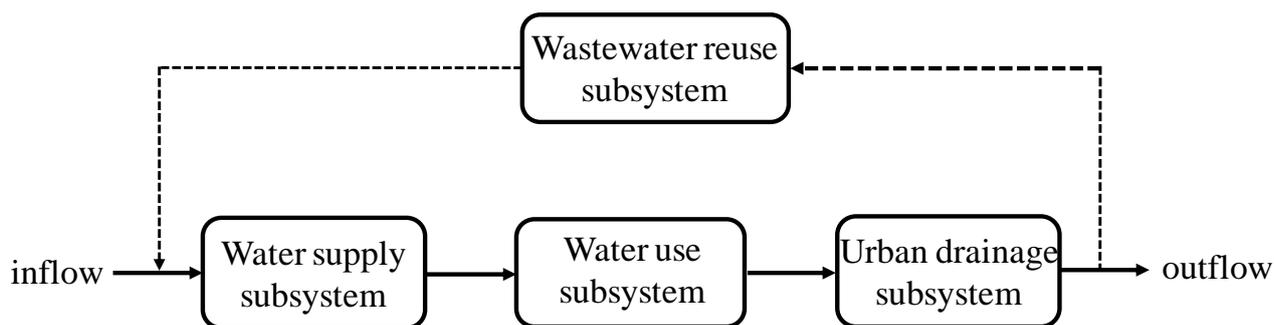


Figure 6 Artificial water cycle (with and without wastewater reuse system)

In order to calculate the entropy change of the artificial water cycle, the hological approach is employed (Aoki, 1989). A subsystem is treatment as a black-box without scrutinizing the internal contents of the subsystem, and the attention is focussed on inputs to and

outputs from a subsystem. The entropy change of the artificial water cycle can be divided into quantitative contribution and qualitative contribution. According to the mass balance, the quantitative contribution of entropy can be obtained, and the treatment process can indi-

cate the quality change about substances in the water flow. Some typical substances can be selected based on the calculation of entropy discussed above and the qualitative contribution of entropy can be calculated.

Ecosystems are conceived as self adapting and self-organization systems (Jørgensen et al., 1998), that they have property of dynamically equilibrium. Since in the equilibrium condition, the internal entropy change $d_i S = 0$, the entropy change of the system is expressed as

$$\Delta S = \Delta_e S = \sum \Delta_e S_N + \sum \Delta_e S_A \quad (7)$$

where, $\sum \Delta_e S_N$ and $\sum \Delta_e S_A$ refer to entropy change from natural water cycle and artificial water cycle, respectively.

The three kinds of entropy changes of UWS are described as follows:

UWS - Natural water cycle:

$$\sum \Delta_e S_N = \Delta_e S_{N1} + \Delta_e S_{N2} + \Delta_e S_{N3} \quad (8)$$

UWS - with wastewater reuse subsystem:

$$\sum \Delta_e S_A = \Delta_e S_{A,S} + \Delta_e S_{A,U} + \Delta_e S_{A,D} + \Delta_e S_{A,R} \quad (9)$$

UWS - without wastewater reuse subsystem:

$$\sum \Delta_e S_A = \Delta_e S_{A,S} + \Delta_e S_{A,U} + \Delta_e S_{A,D} \quad (10)$$

CONCLUSIONS

Two conceptual models to analysis the UWS based on entropy were established. Model 1 is considered natural UWS as internal part, while natural water cycle is external contribution in model 2.

In model 1, the entropy increase of the natural UWS is equal to zero, so the entropy change of the UWS is the entropy change by the artificial water cycle. Through the water balance and purification reactions of j kinds of typical pollutants in the UWS, the entropy change of disturbance on water quantity and disturbance on water quality for artificial water cycle can be calculated.

In model 2, the entropy change of the UWS is a sum of the entropy change by the natural water cycle and the artificial water cycle. The meteorological and hydrological data together with mass balance and treatment process analysis are essential for calculating the entropy changes of UWS.

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