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Development of Method for Assessing Water Footprint Sustainability

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Abstract: Large scale production of water-intensive industrial products can intensify water scarcity, resulting in potential unsustainable water use at local and regional scales. This study proposes a methodological framework for assessing the *WF* sustainability of multiple interdependent products in a system, and one of China's four major large modern coal chemical industry bases is used as a case study. A Mixed-Unit Input-Output (MUIO) model was applied to calculate the blue water footprint (*WF*) for 19 major coal-based energy and chemicals in the study area, based on which the *WF* sustainability of production of the products were assessed using different indicators. Technical coefficient matrix and direct water consumption vector of the products were constructed based a database that were built by field research in the study area. Accounting result indicates that the blue *WF* of the coal-based products range from 2.5×10^{-4} m^3/kWh for coal-fired power to 55.25 m^3/t for Polytetrahydrofuran. The sustainability assessment reveals that the blue *WF* of all products produced in the study area are sustainable at both product and regional levels, while over half of them have reached the advanced level. However, the blue *WF* of a few products with large production capacities has just crossed the sustainable thresholds, posing potential threat to the local environment. This paper concludes with a discussion on the choice of blue *WF* accounting approach, methods to promote *WF* sustainability of coal-based products, and suggestions for the *WF* management in general.

Keywords: water footprint; sustainability assessment; *WF* accounting method; coal-to-chemicals; water scarcity weighted *WF*; sustainability indicators

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1. Introduction

Water scarcity can cause severe socio-economic consequences from local to global scales [1,2]. The World Economic Forum rated water crises as one of the major global risks over the next decade [3]. Energy and chemical industry is one of the largest water consumers; it demonstrates high water sensitivity because each stage of the entire life cycle of its productions needs water (e.g., mining or extraction, processing and conversion) [4]. The International Energy Agency projected a rise of 60% in global water consumption for primary energy production and power generation through 2040 [5]. In China, the energy and chemical uses have dramatically increased in last decades due to rapid economic expansion. Consequently, China released the Energy Production and Consumption Revolution Strategy (2016–2030), which set up a series of targets for 2030 including the share of non-fossil fuel in the energy mix, and the nation's energy self-sufficiency rate [6]. However, coal-based energy will continue to form the major part of China's energy mix over the next decade due to the low cost and the abundance of domestic reserves [6].

There are two major problems exist in China's fossil energy resources endowment. First, the energy structure of China is characterized by "rich coal, meager oil, and little gas"; the proven reserves are comprised of 94% coal, 5% crude oil, and 0.6% natural gas [7]. China now has become the world's largest and second largest importer of crude oil and natural gas, respectively [8]. The dependence of imported energy and chemicals poses a great threat to China's energy and chemicals supplies. Second, the distributions of coal and water resources are severely mismatched across the country's territory. Nearly 70% of coal production is concentrated in the northern and western provinces, that only account for 6.5% of China's total water resources, making water a significant vulnerability in the country's energy and chemical supplies [9]. To cope with these problems, China gave great priority to the development of 14 large coal energy bases and four large modern coal chemical industry bases during its 12th and 13th Five-Year periods (2011–2020). To reduce its dependence on foreign petroleum, China also made great efforts to develop technology to convert abundant coal into clean fuels and value-added chemicals [10]. However, producing coal-based fuel and chemicals in these coal-rich water-limited energy bases has been controversial due to the high water-consuming processes. Large-scale water-intensive industrial production within an industrial base potentially threat the local environment. Thus, life cycle assessments related to water scarcity for the arid industrial bases in China is of great importance to achieve environmental sustainability.

Water footprint (*WF*) can be used as an indicator of environmental sustainability in water use. The *WF* concept was first introduced in 2002 by [11]; it functions as a multidimensional indicator of freshwater use (i.e., blue *WF* and green *WF*) and pollution status (i.e., gray *WF*) [11–13]. The Water Footprint Network (*WF*N) community considers *WF* as a volumetric metric and focuses on the consumptive freshwater use. Simultaneously, the Life Cycle Assessment (LCA) community converts *WF* into an environmental impacted-oriented indicator by a weighting scheme called characterization, which is recommended in ISO document 14046 on *WF* [14]. Over the past decade, researchers in the two communities have given rise to a debate over so-called better *WF* accounting approach [15–21]. Nevertheless, there is no contradiction in fundamental principles of the methods proposed by two sides; information provided by volumetric *WF* and impacted-oriented *WF* should be complementary rather than competing [22], and the choice of the two *WF* accounting depends on the purpose of a study.

Previously, the *WF*N-*WF* has been adopted in studies focusing on the optimal water resources allocation and productivity of freshwater use [10,23,24], whereas LCA-based *WF* accounting using input-output (IO) approach has been used in assessing the potential environmental impact of products [4,25–28]. The IO framework are extensively used to estimate the *WF* of industrial sectors at global scale (e.g., [29,30]), national or multiregional scale (e.g., [31–36]), and basin scale (e.g., [37–40]), but rarely used to assess the potential impact of the production of interdependent products at local or sub-local scales, because IO tables are compiled only at national or provincial levels due to cost and resource constraints. This study attempts to fill in this research gap by introducing a methodological framework for assessing the *WF* sustainability of multiple interdependent products in a system. The Mixed-Unit Input-Output (MUIO) model is adopted in the framework to account *WF* of the products, and three sustainability assessment indicators are then proposed. A large modern coal chemical industry base in Northwest China is used as a case study. Technical coefficient matrix and direct water consumption vector for the products in the study area were constructed based on a database, which was built by our research team through on-site survey and investigation. Since zero liquid regulation has been enacted in China's major arid industrial bases, the assessment was conduct at product and regional levels with a focus merely on blue *WF*.

2. Methods

2.1. The Blue WF Assessment Framework

The blue *WF* assessment of a framework is proposed in this section. The overall methodology of the *WF* assessment is shown in Figure 1. The first phase of the proposed framework is the scope setting, which determines the major industrial products that are considered in the assessment. This phase also includes the analysis of the interdependence among the products. The functional unit of *WF* for each product should then be decided in this phase. The second phase is data collection in the region where the products are produced, preliminary analysis of the data can be conducted. In the third phase of the framework, the technical coefficient matrix, and the direct water consumption vector for the are constructed based on the data collected. The coefficient matrix is a p-by-p matrix that describes the interdependence between products within the scope of the study determined in phase one, and the direct water consumption vector is a p by 1 vector contains the direct water coefficients for each product. The accounting model then is built in the fourth phase, followed by *WF* sustainability assessment of the interdependent products at product scale and regional scale.

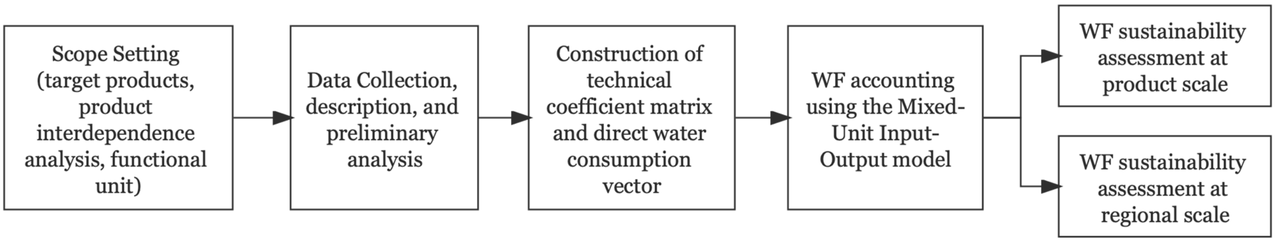

Figure 1. The general framework for the *WF* sustainability assessment.

2.2. Blue WF Accounting Model

The MUIO model is employed to account the blue *WF* of each coal-based energy and chemical product. The MUIO model is a top-down framework used for environmental life-cycle analysis; it was first introduced by Hawkins et al. [28]. The MUIO model in the form of *WF* can be expressed in Equation (1) shown below:

$$\sum_{n=1}^{P} WF_n = \sum_{n=1}^{P}\sum_{m=1}^{P} a_{nm} WF_n + \sum_{n=1}^{P} dw_n \tag{1}$$

where WF_n represents the blue *WF* of the nth product; a_{nm} is the technical coefficient, which represents the amount of product m directly consumed for producing unit product n; dw_n indicates the direct water use coefficient of product n. P is the total number of major products in the system. a_{nm} and dw_n are computed using Equation (2):

$$a_{nm} = \frac{\sum_j z_{nm}^j}{\sum_i x_n^i}; dw_n = \frac{\sum_i w_n^i}{\sum_i x_n^i} \tag{2}$$

where z_{nm}^j is the total amount of product m flows from the jth enterprise for the production of product n during a time period; x_n^i is the total amount of product n produced in the ith enterprise during the same period; w_n^i is the total freshwater consumed for producing product n in the ith enterprise during the period. Equation (1) can be further expressed in matrix terms as follows:

$$DW = (I - A)WF \tag{3}$$

where WF represents the vector containing blue WF of each products; I denotes an identity matrix; A and DW represents the technical coefficient matrix and the direct freshwater consumption vector, respectively, which are in the form shown below.

$$A = \begin{bmatrix} a_{11} & \cdots & a_{1m} & \cdots & a_{1p} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nm} & \cdots & a_{np} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{p1} & \cdots & a_{pm} & \cdots & a_{np} \end{bmatrix}; DW = \begin{pmatrix} dw_1 \\ dw_2 \\ \vdots \\ dw_n \\ \vdots \\ dw_p \end{pmatrix} \quad (4)$$

WF can then be calculated by the MUIO model as Equation (5):

$$WF = (I - A)^{-1} DW \quad (5)$$

where $(I - A)^{-1}$ is called the Leontief inverse matrix. The indirect water use coefficient vector can be calculated by abstracting DW from WF, shown in Equation (6).

$$IDW = WF - DW \quad (6)$$

where IDW denotes the vectors containing indirect freshwater water for each product.

2.3. Blue WF Sustainability Assessment

The sustainability assessment of *WF* of a product is twofold: the blue *WF* assessment against a reference standard, and the *WF* assessment against the regional water availability. The former indicator given in Equation (7) can be used to evaluate the overall technology level of existing industrial plants in terms of water, energy and material conservation.

$$WSSI_p = \frac{WF_p}{WF_p^{ref}} \quad (7)$$

where $WSSI_p$ denotes the *WF* sustainability index based on any reference standard; WF_p^{ref} denotes the blue *WF* of product p under any reference level of technology. In this study, two references are applied: the blue *WF* of product p using the general standard (WF_p^{ref-1}) and using the best practicable technology (BPT) (WF_p^{ref-2}). The current technology is considered unsustainable if both $WSSI_{p-1}$ and $WSSI_{p-2}$ are greater than 1, sustainable if $WSSI_{p-1}$ is less than 1 while $WSSI_{p-2}$ is greater than 1, advanced if both $WSSI_{p-1}$ and $WSSI_{p-2}$ are not greater than 1 (Table 1).

Table 1. Water footprint sustainability assessment methods at product and regional levels.

Assessment Level	Indicator Values	Assessment Results
Product-level	$WSSI_{p-1} > 1$, $WSSI_{p-2} > 1$	unsustainable
	$WSSI_{p-1} \leq 1$, $WSSI_{p-2} > 1$	sustainable
	$WSSI_{p-1} \leq 1$, $WSSI_{p-2} \leq 1$	advanced
Regional-level	$WSRI_{p-1} > 1$, $WSRI_{p-2} > 1$	unsustainable
	$WSRI_{p-1} \leq 1$, $WSRI_{p-2} > 1$	sustainable
	$WSRI_{p-1} \leq 1$, $WSRI_{p-2} \leq 1$	advanced

The second indicator given in Equation (8) takes into account both the technology level and the regional water resources endowment. That is, a product produced at the same technology level is considered as sustainable in water abundant region does not necessarily means that it is also sustainable in regions where water resources are scarce.

$$WSRI_p = \frac{WSI \cdot WF_p}{WF_p^{ref}} \tag{8}$$

where $WSRI_p$ denotes the WF sustainability index for product p at regional level. WSI is the regional water stress index. Similarly, the current technology is considered unsustainable at regional level if both $WSSI_{p-1}$ and $WSSI_{p-2}$ are greater than 1, sustainable if $WSRI_{p-1}$ is less than 1 while $WSSI_{p-2}$ is greater than 1, advanced if both $WSSI_{p-2}$ and $WSSI_{p-2}$ are not greater than 1 (Table 1). The WSI index is defined by the ratio of total annual freshwater withdrawals to hydrological availability, it was modified by [41] to differentiates watersheds with strongly regulated flows. Later, Ref. [42] computed WSI for China's provinces and major river basins using ArcGIS 10.0.

Finally, to assess the overall sustainability of production in a industrial base, the weighted sum WF sustainability index for all products at regional level is computed as Equation (9).

$$WSRI = \frac{\sum_{p=1}^{P} WSRI_p \cdot CAP_p \cdot WF_p}{\sum_{p=1}^{P} CAP_p \cdot WF_p} \tag{9}$$

where $WSRI$ denotes the overall WF sustainability index for industrial base at regional level, CAP_p denotes the total production capacity of product p in the base. Water footprint sustainability indicators and their abbreviations and measurement units are shown in Table 2.

Table 2. Water footprint sustainability indicators and their abbreviations and measurement units.

Indicators	Abbreviations	Measurement Units
Water footprint	WF	m^3/t or m^3/kWh
Blue water footprint	Blue WF	m^3/t or m^3/kWh
Water sustainability index at product level based on general standard	$WSSI_{p-1}$	unitless
Water sustainability index at product level based on BPT	$WSSI_{p-2}$	unitless
Water sustainability index at regional level based on general standard	$WSRI_{p-1}$	unitless
Water sustainability index at regional level based on BPT	$WSRI_{p-2}$	unitless
Overall sustainability of production in a industrial base	$WSRI_{Base}$	unitless

3. Case Study

3.1. The Ningdong Base

The Ningdong Energy and Chemical Industry Base (Ningdong Base, Ningxia, China) in Ningxia Hui Autonomous Region of China is chosen as a case study. Ningxia is covered in arid and semi-arid climate; the annual average precipitation is 289mm while the annual average evaporation is 1250 mm [43]. Ningdong Base is one of the 14 national major large-scale coal bases and four national major coal-to-chemical industry bases in China, making it an ideal industrial base for the analysis. By the year of 2020, many state-owned and private large enterprises have invested more than 60 coal mining, coal-fired power and advanced coal chemical projects in the base, including the world's largest single CTL project (Table 3). The annual total capacities of coal mining, coal-fired power generation, and chemical production have reached 90 million tons, 15,660 MW, and 25 million tons, respectively. The massive production of coal, coal-fired power, and coal-based products in Ningdong has intensified the water stress of the province. It is reported that over 250 million cubic meter of freshwater is consumed annually in the base [43].

Table 3. Statistics of the coal-based energy and chemicals in the Ningdong Base (2020).

Product	Abbreviation	No. of Enterprises	No. of Projects	Total Capacity (10^4 ton/a)
Washed coal	COAL	2	13	9000
Coal-fired electricity	ELEC	10	15	15,660 (MW)
Coal-to-liquid	CTL	1	1	400
Coal-to-methanol	CTM	3	4	175
Goal gas to methanol	CGTM	2	2	45
Coke	COKE	2	3	590
Goal gas to olefin	CGTO	1	1	60
Methanol to olefin	MTO	3	5	205
Dimethyl ether	DME	1	1	21
Polyoxymethylene	POM	2	2	11
Ammonia	NH_3	2	2	55
Urea	UREA	1	1	70
Calcium carbide	CaC_2	1	1	115
Acetylene	ACET	1	1	30
1,4-Butanediol	BDO	1	1	20.8
Polytetrahydrofuran	PTMEG	1	1	9.2
Acetic acid	ACA	1	1	30
Vinyl acetate	VAC	1	1	40
Polyvinyl alcohol	PVA	1	1	10

3.2. *Blue WF Accounting for the Products*

Prior to *WF* accounting for the products, the technical coefficient matrix and direct water use a vector for the main products in an industrial base need be constructed. In this study, we conducted field research to collect first-hand data in the Ningdong Base, during which our research team conducted site visits and interviews in many major ongoing coal mines, coal-fired power stations, and coal-to-chemical projects in Ningdong. Because the number of projects for some products are more than one, the weighted averaged values for unit water, energy and raw material consumption based on the production capacity of the projects were computed to represent the overall technical level of the product in the Base. The technical coefficient matrix and direct water use vector for major products in Ningdong is shown in Table 4, in which the unit for electricity consumption is kWh/t (kWh/kWh for power self-consumption) and t/t for material consumption (t/kWh for electricity); the unit for water consumption is m^3/t (m^3/kWh for electricity).

Table 4. The technical coefficient matrix and direct water consumption vector for major products in the Ningdong Base.

Technical Coefficient Matrix																			
Products	COAL	ELEC	CTL	CTM	CGTM	COKE	CGTO	MTO	DME	POM	NH3	UREA	CaC2	ACET	BDO	PTMEG	ACA	VAC	PVA
COAL	0	0.0003	2.230	1.926	0	1.175	2.960	5.10	2.12	2.00	1.61	0	0	0	0	0	0	0	0
ELEC	18.29	0.05	1078.37	363.68	151.95	44.06	848.61	2680.0	80.0	990.0	505.46	78.52	3262.2	206.96	918.49	869.41	91.63	162.15	696.20
CTL	0.0001	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CTM	0	0	0	0	0	0	0.253	0	0	0	0	0	0	0	1.215	0.057	0.538	0	0.873
CGTM	0	0	0	0	0	0	0.253	0	0	0	0	0	0	0	1.215	0.057	0.538	0	0.873
COKE	0	0	0	0	0	0	0	0	0	0	0	0	0.686	0	0	0	0	0	0
CGTO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MTO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
DME	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NH_3	0	0	0	0	0	0	0	0	0	0	0	0.571	0	0	0	0	0	0	0
UREA	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CaC_2	0	0	0	0	0	0	0	0	0	0	0	0	0	3.813	0	0	0	0	0
ACET	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.282	0	0	0.325	0
BDO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.490	0	0	0
PTMEG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ACA	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.710	0
VAC	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.819
PVA	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Direct water consumption vector																			
Freshwater	0.122	0.00022	9.55	11.13	4.19	1.05	15.91	14.05	7.30	5.76	10.89	2.13	0.81	4.57	18.40	6.74	1.93	2.83	16.53

The blue *WF* accounting is then conducted using the MUIO model based on the technical coefficient matrix and direct water use vector. The blue *WF* results are shown in Figure 2. It shows that the blue *WF* of different coal-based energy and chemicals differ significantly. The standard deviations of the direct water, indirect water, and *WF* of the products are 5.98, 12.24, and 14.83 m^3/t, respectively. In general, the blue *WF* of products at the downstream are greater than that of the upstream products. The average blue *WF* of electricity in the study area is 2.51×10^{-4} m^3/kWh. The washed coal in the study area has an average blue *WF* value of 0.126 m^3/t. CaC2 and COKE both have relatively small values of *WF*. The coal-based chemicals at the downstream such as BDO, PVA, and PTMEG require a large quantity of freshwater along their production chain. For example, the blue *WF* of PTMEG is 55.25 m^3/t, which means over 55 tons of freshwater is consumed for producing one single ton of PTMEG. It is worth mentioning that methanol produced using alternative routes can result in significantly different *WF* values. The blue *WF* of methanol based on the CTM route (11.65 m^3/t) is over 2.75 times greater than that using the CGTM route (4.23 m^3/t). Likewise, the blue *WF* of olefin based on the MTO route is 15.37 m^3/t, while it is 18.12 m^3/t using the CGTO route.

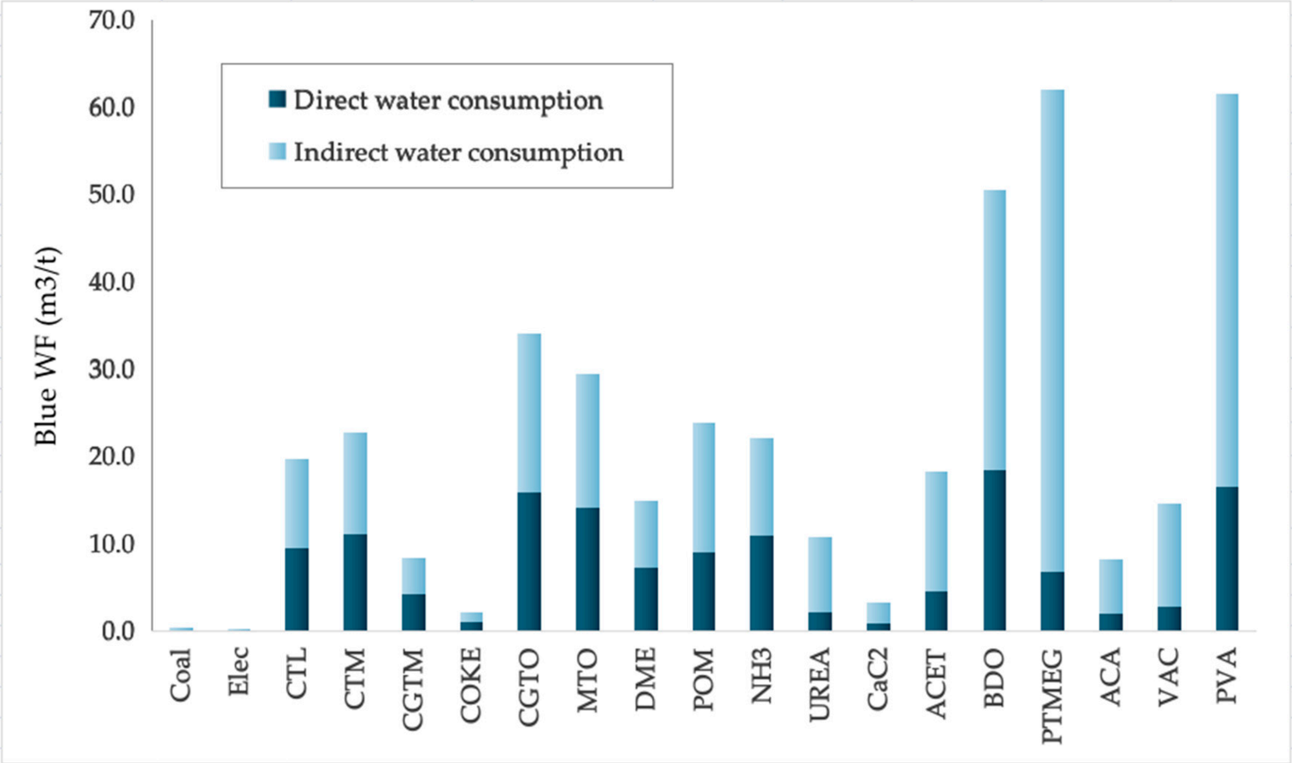

Figure 2. Blue *WF* of the coal-based energy and chemicals in the Ningdong Base.

The analysis for the structure of *WF* can help to find the major contributor of the total *WF*, it was therefore analyzed in the study. Figure 3 presents the distribute proportion of direct and indirect *WF* for each product. The proportion of indirect *WF* in the total *WF* covers a wide range, from 0.9% for CGTM to 87.8% for PTMEG. The standard deviation of the proportion of direct *WF* is 31.62%. Among the products, the direct water consumption of CTL, CTM, CGTM, COKE, MTO, DME, and NH_3 accounts for more than 90% of the total *WF*. Most of the above-mentioned products are secondary products synthesized directly from coal. On the contrary, the tertiary and quaternary products from coal have much smaller percentage for direct water consumption. For example, the direct water stands for 12.2 to 36.78% for VAC, PVA, and PTMEG.

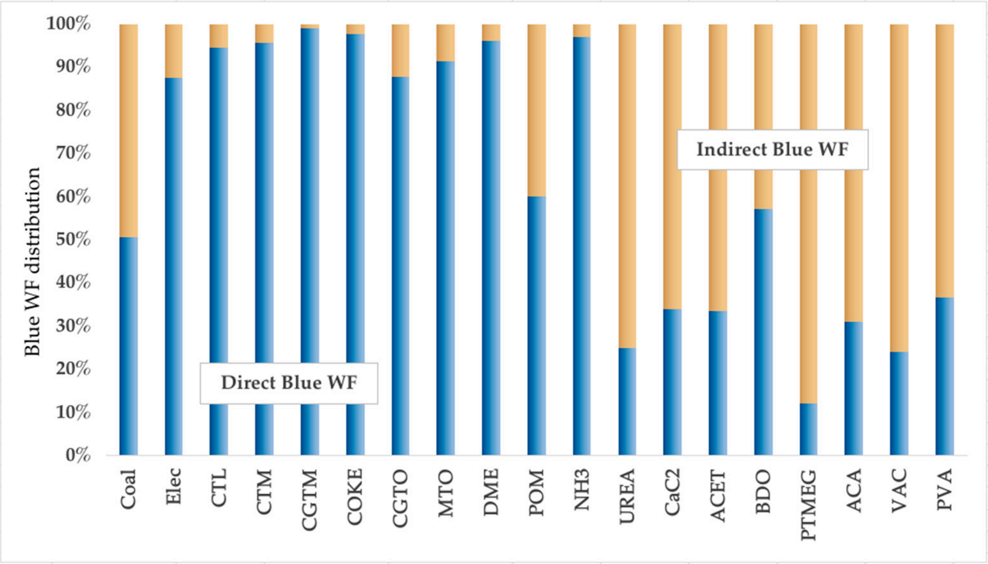

Figure 3. Blue *WF* distribution proportion of the coal-based products in the Ningdong Base.

3.3. Validation of the Accounting Model

The *WF* of the same industrial product based on different production routes can be significantly different. Even with the same production route, the difference in *WF* can still be remarkable due to different level of water-saving, energy-saving, and material consumption technologies adopted. Thus, validation of the *WF* accounting model needs be conducted with the same products produced at the same sites. In the current study, the *WF* accounting model is validated by comparing the blue *WF* of the coal-based products calculated by the proposed model with the blue *WF* of the same products produced in Ningdong, which were accounted by a process-based model reported in literature [10]. Figure 4 illustrates the comparison results. It shows that the blue *WF* of the two models are consistent, with R^2 of 0.906, Pearson correlation coefficient (PCC) of 0.952, and normalized root mean squared error (NRMSE) of 0.112 m^3/t. The results indicate the good performance of the *WF* accounting model.

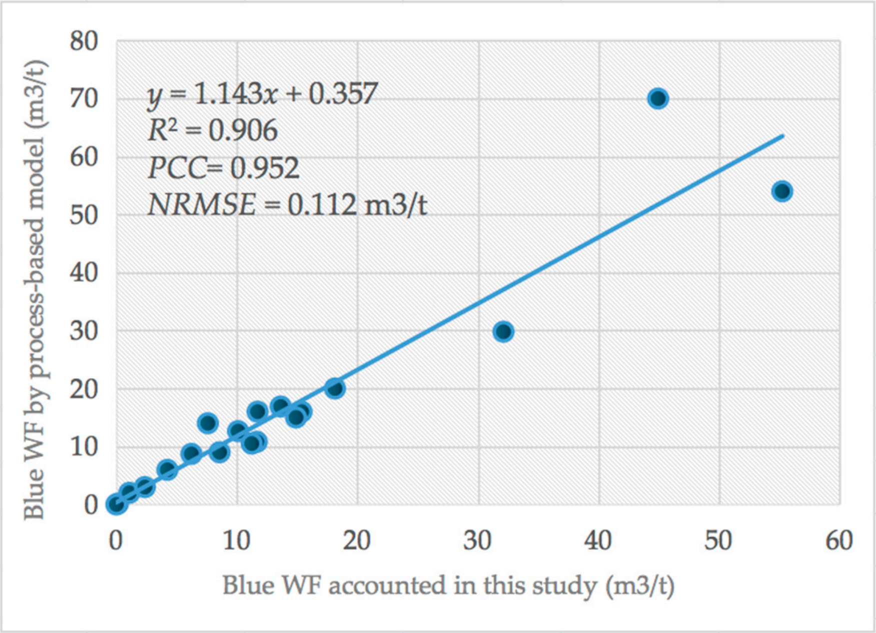

Figure 4. Comparison of blue *WF* of products from the MUIO model verse a process-based model.

3.4. Blue WF Sustainability Assessment

3.4.1. Standards and Norms

To assess the blue *WF* sustainability of the coal-based energy and chemicals at two different levels, the product *WF* under referenced level of technology needs be computed. China has issued a serial of national standards of water intake and energy consumption for power generation and major chemical productions [44–51]. In addition, updated standards and norms have recently been issued by the provincial government [52]. The standards of water and coal consumption for power generation differ with installed unit capacity (Table 5). The norms for water and energy consumption for washed coal and other chemicals are shown in Table 6. The analysis does not include the chemicals of which national or provincial standards are not issued.

Table 5. Standard quantity of water and coal consumption for unit rated capacity.

Cooling System	**Freshwater Consumption for Install Unit Capacity (m^3/MWh)**		
	<300 MW	**300 MW~500 MW**	**$\geq$600 MW**
Circulating	3.20	2.75	2.40
DC cooling	0.79	0.54	0.46
Air cooling	0.95	0.63	0.53
Level	Coal consumption for unit of 600 MW (tce/MWh)		
	Subcritical	Supercritical	Ultra-supercritical
Standard	0.319	0.306	0.293
Advanced	0.313	0.298	0.288

The conversion coefficient to standard coal equivalent is 0.1229 tce/MWh.

Table 6. Standard quantity of water and coal consumption for coal and chemicals.

Product	**Freshwater Consumption (m^3/t)**		**Energy Consumption (tce/t)**	
	General	**Advanced**	**General**	**Advanced**
COAL	0.34	0.26	0.007	0.003
CTL	10	7	2.5 *	2.2 *
CTM	15	9	2.2 *	1.8 *
CGTM	15	9	1.65 *	1.3 *
COKE	1.4	1.2	0.155	0.127
MTO	15	12	4.5	3.7
DME	11	–	1.225	1.146
POM	24	–	2.8 *	2.1 *
NH3	14	10	4	3
CaC2	1.1	–	3.2 *	3.05 *
ACET	2.1	–	–	–
BDO	23.8	–	1.5	0.95
ACA	3.2	–	0.429	0.3
VAC	8	–	0.565	0.41
PVA	10.9	–	2.75	2.072

* The ones marked with star indicate that the material coal consumption is also included.

3.4.2. Blue WF under General Standard and the BPT

Prior to the computation of $WF_p{}^{ref}$ for the energy and chemical products, one should update the technical coefficient matrix and direct water use vector using the data in the general standards and the BPT, to compute the *WF* under general standard and the BPT, respectively. In the study area, there are 15 coal-fired power stations in operation, which include 31 installed units. The average capacity of the power stations is 1044 MW, whereas the average capacity of installed units is 505 MW. To compute the $WF_p{}^{ref}$ of electricity, the values in the norms corresponding to $\geq$500 MW for water consumption and 600 MW for coal consumption were adopted. Ideally, the $WF_p{}^{ref}$ is computed with referenced water, energy and materials consumption. However, only a few products have referenced raw material consumption. For example, the scope of energy consumption standards for CTL and CTM covers both thermal coal and material coal consumption. It should be noted that the energy consumption standards are given based on coal equivalent (7000 kcal/kg), thus one needs to convert the actual energy consumption into coal equivalent. The $WF_p{}^{ref}$ versus actual *WF* of the coal-based energy and chemicals are shown in Figure 5.

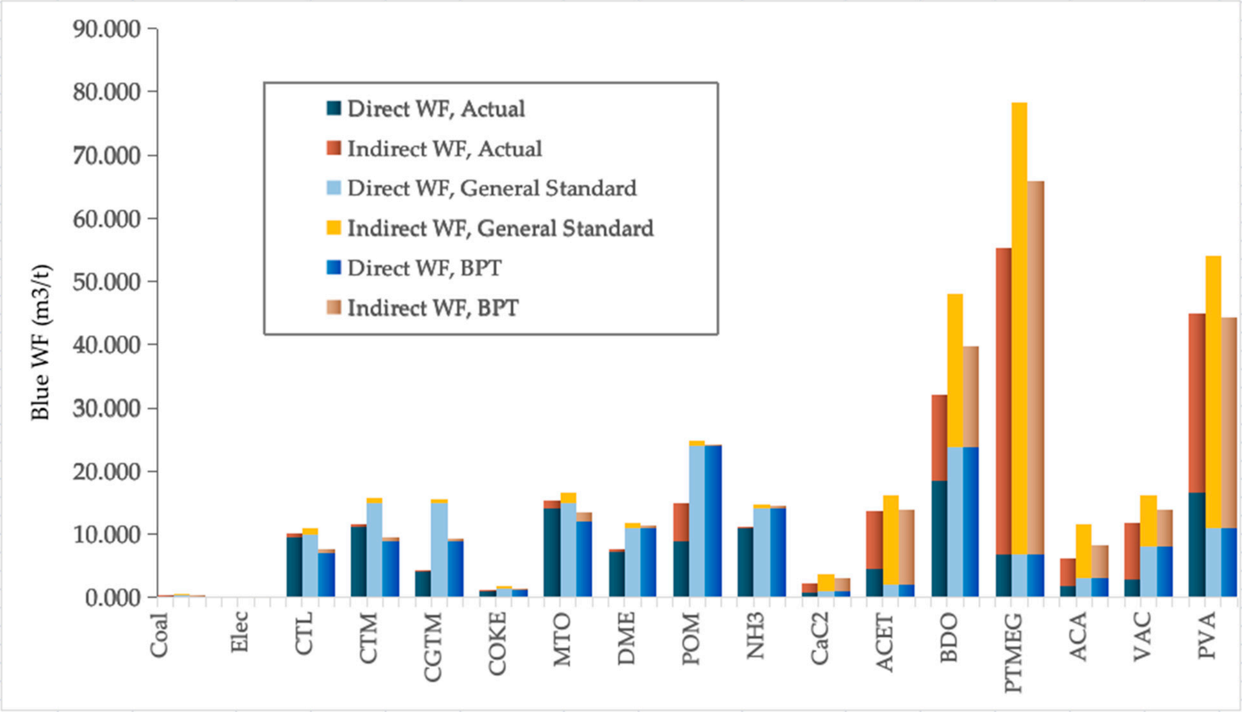

Figure 5. Actual blue *WF* versus blue *WF* under general standard and the BPT in the Ningdong Base.

3.4.3. Blue WF Sustainability Indicators

The blue *WF* sustainability assessment indicators at product and regional levels were computed and shown in Figure 6. Result shows that all products manufactured in the Ningdong Base are sustainable at both product and regional levels. At the product level, the technology of 12 products has reached the advanced level, which includes the primary energy of coal and secondary energy of coal-fired electricity. NH_3 and PVA are very close to the advanced level, with $WSRI_{p-1}$ values of 1.075 and 1.016, respectively. CTL and MTO have just crossed the sustainable thresholds, with $WSRI_{p-1}$ values of 0.921 and 0.928. At the regional level, the technology of most of the products have reached the advanced level in terms of *WF*, whereas CTL, CTM, and MTO are close to the advanced thresholds. Considering the production capacity of the energy and chemical products, the overall *WSRI* value of the Ningdong Base is 0.876 based on *WF* under the BPT. This means that the Ningdong Base is sustainable and advanced in terms of water consumption. It is noteworthy that, methanol produced based on the CGTM route is much smaller than that based on the CTM route. The $WSRI_{p-1}$ value of the latter is 2.71 times greater than that of the former.

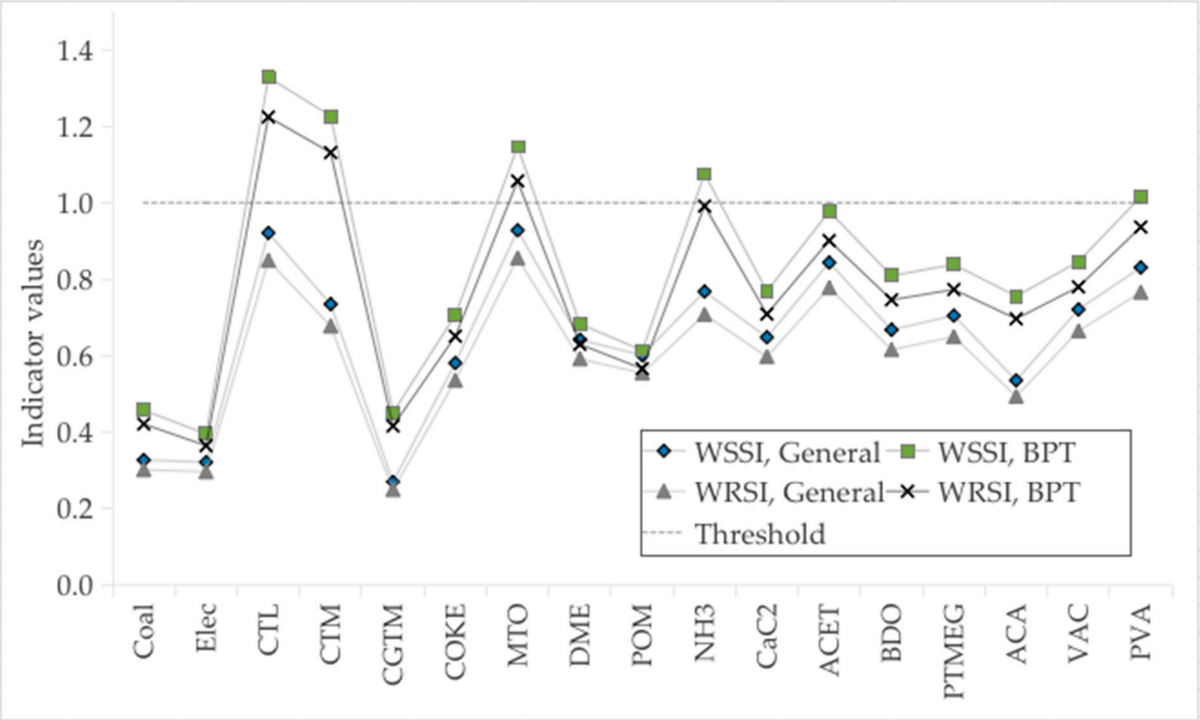

Figure 6. WSSI and WRSI based on general standard and the BPT in the Ningdong Base.

4. Discussion

4.1. Volumetric WF versus Impacted-Oriented WF

The choice of *WF* accounting approach depends on the goal of a study conducted. The *WFN-WF* is more preferable for studies in the water resources management, especially in the efficiency, sustainability, and equability of water resources allocation and the productivity of freshwater use [10,23,24]. LCA-based *WF*, on the other hand, is more appropriate for assessing the potential environmental impact of different products or alternative production processes at different levels, especially when regional water availability is considered [4,25–27]. Our study adopted the LCA-based *WF* to assess the sustainability of different coal-based energy and chemicals at product and regional levels. Results indicate that, as one of the national modern coal chemical industry bases, the wastewater treatment, recycling, and reuse technologies that have widely adopted in the base have offset the intensified water scarcity that would have been caused by the large-scale industrial production. However, further *WF* reducing measures should be implemented in some major projects in the industrial base; investment in technical improvement in the process unit with lower water, energy requirements is highly encouraged. For example, the CTL project, which is regarded as the “No. 1 Project ” of Ningxia Province, has relatively large product *WF* comparing to that of other projects in the base. Likewise, there also exist a gap between the average level of *WF* of the MTO projects in the base and the advanced level. Furthermore, more frequent use of byproducts of upstream can reduce the potential environmental impact of large-scale production. For example, the use of coke oven gas, a main byproduct of COKE, for the methanol production may enhance the environmental sustainability of an industrial base.

4.2. Improve the Sustainability

As one of the nation’s major modern coal chemical industry bases, Ningdong has launched a comprehensive control system for energy and water conservation and environmental protection. We, thus, expected that the water-saving and energy-saving technologies adopted for production of the products in Ningdong are superior compared to their corresponding national average. Obviously, the results of the *WF* sustainability analysis is consistent with our expectation. According to the on-site data we collected, the average wastewater reuse rate of production of the major products is 34.18%; it is contributed by 15 reclaimed water treatment plants with a total capacity of 3.52×10^5 m^3/d in the study area. In addition, three pit water treatment plants in the base with a total capacity of 1.2×10^5 m^3/d are also in operation. A question is whether pit water use should be included in the *WF* accounting. In our analysis, the use of pit water was excluded considering that (1) pit water is mainly interstitial water collected along with mining and cannot be used as water resources without proper treatment; (2) direct discharge of the metal-rich pit water is a great threat to the environment. In the study area, the product *WF* would be 17.02% to 104.4% greater if the use of reclaimed water and pit water were substituted with freshwater, which would lead to unsustainable production for majority of the products. For example, the *WF* of COAL and CTL would be 0.245 m^3/t and 20.64 m^3/t, respectively, if only freshwater were used. Therefore, besides the efficiency improvement of water, energy, and material use, increasing the ratio of nontraditional water use is also an important method to enhance the *WF* sustainability. In fact, according to a recent water utilization plan in Ningxia [53], the Province proposes to substantially increase the utilization of nontraditional water resources. The plan clearly stated that, by the year of 2025, the utilization rate of reclaimed water and pit water shall reach 50% and 90%, respectively [53].

4.3. Enhance the Life-Cycle Thinking for Water Management

In the recent years, China's central and local authorities have issued serious of regulations and plans to improve the conservation and utilization of water resources in water scarcity basins [53,54]. A very recent plan released by five China's ministries set clear goals for the establishment of rigid restraint system of water resources, promoting water conservation, utilization of unconventional water resources, etc. Meanwhile, the Ministry of Water Resources of China lately claimed that a national water quota system has been basically established. This system covers water quotas for 105 products, including 70 industrial products. However, all the hard efforts that have been made were solely in direct water utilization, neglecting the importance of indirect water use along the supply chains. Consequently, the analysis on water consumption can be incomplete. In the case study, the *WF* of all energy and chemical products produced are sustainable, which would lead to inconsistent results if only direct water consumption were considered. For example, the direct water consumption for PVA in Ningdong is 16.53 m^3/t, which exceeds its general standard of 8 m^3/t and will be determined as unsustainable. This inconsistency is due to the fact that the relatively-high efficient use of energy and materials in the PVA production process, as well as the efficient water use of the upstream production compensate the inefficient freshwater consumption in the PVA production process. These results further address the necessity of life-cycle thinking (LCT) for water resources management, which seeks to identify water use improvement opportunities at all stages across the life cycle. The LCT can provide a comprehensive approach in support of the overall reduction of environmental impacts in water resources utilization.

4.4. Establishment of National WF Benchmarks

The purpose of *WF* sustainability studies generally can be grouped into two categories: (1) assessing whether the *WF* of a product unnecessarily contributes to global, national, regional or local *WF* of humanity and (2) assessing whether the *WF* contributes to specific hotspots [55]. The interest of our study lies in the former one, which compares each separate product *WF* with a benchmark for that product. However, although we have established *WF* benchmarks, they were merely based on norms of water and coal consumption for power generation, and the standards of water and energy consumption for washed coal and other chemicals. The standards of materials consumption for most of the products were not considered simply because such standards do not exist. The limitation of the current study reveals the necessity of establishment of standardized national or regional *WF* benchmarks in China, especially for the major products in the water-intensive coal-to-chemical industry.

The *WF* benchmark values can be used as instruments to evaluate the advancement of specific production technology, set criteria for newly invested production capacity, as well as formulate *WF* reduction targets. Reference [56] introduced a set of global *WF* benchmarks for over 120 agricultural products, but the literature lacks studies on *WF* benchmark setting for industrial products. In addition, the result of the current study also suggests that the regionalization and industrial technology consideration are necessary for the establishment of such benchmarks. That is, the level of regional or local water scarcity, and the choice of different industrial routes should also be fully considered in future the analysis.

5. Conclusions

This study attempts to fill in a current research gap by introducing a methodological framework for assessing the blue *WF* sustainability of multiple interdependent products in a system. The Mixed-Unit Input-Output (MUIO) model is adopted in the framework to account *WF* of the products, and three sustainability assessment indicators are then proposed. A large modern coal chemical industry base in Northwest China, in which 19 major coal-based energy and chemical products are produced is used as a case study. Technical coefficient matrix and direct water consumption vector for the MUIO model were constructed based on first-hand data collected by on-site field research in the study area, after which *WF* accounting and sustainability assessment were conducted at product and regional levels. The conclusions drawn from the proposed framework, as well as from the results and discussion of the real-world case are as follows: (1) although the top-down approach is usually applied to investigate the interdependent among industry sectors in terms of water consumption, our method has generalized it to calculate the blue *WF* of multiple interdependent products. The validation results indicate the good performance of the model. (2) Instead of using the IO tables that are directly compiled at national or provincial levels for regional and global scale *WF* analysis, the proposed method usually requires on-site data collection and computations, based on which the technical coefficient matrix and direct water consumption vector of the products are constructed. (3) In the case study, the blue *WF* of the coal-based products differ significantly. The standard deviation of the blue *WF* of the products in the study area is 14.83 m^3/t, to which the indirect water contributes much more than direct water. (4) Generally, lowering the indirect water use is the key to *WF* reduction for the downstream products whereas lowering direct water use is more important for the upstream product *WF* reduction. (5) Although the blue *WF* of all products manufactured in the study area are sustainable at both product and regional levels, further *WF* reducing measure should be implemented for several major products such as CTL and MTO. (6) To enhance the blue *WF* sustainability, the ratio of nontraditional water resources to total water use should also be further increased. (7) The LCT should be adopted to provide a comprehensive approach in support of the overall reduction of environmental impacts in water resources utilization in China’s arid coal bases. (8) It is suggested to establish standardized national or regional *WF* benchmarks for the major products in the water-intensive coal-to-chemical industry.

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