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2 Water-energy-food nexus: concepts, questions and methodologies

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9

10 **Abstract**

11 The water-energy-food nexus has gained increasing attention in the research  
12 communities as the security of water, energy and food becomes a very high concern  
13 due to future uncertainties. Studies pertaining to calculations of flows and dependencies  
14 between different resources, assessments of technology and policy applications, and  
15 quantifications of system performance have been conducted to understand their  
16 interlinkages and develop management options. This paper provides a state-of-the-art  
17 review on the concepts, research questions and methodologies in the field of water-  
18 energy-food. First, two types of nexus definition are compared and discussed to  
19 understand the nature of nexus research issues. Then, nexus research questions are  
20 summarized into three themes: internal relationship analysis, external impact analysis,  
21 and nexus system evaluation. Eight nexus modelling approaches are discussed in terms  
22 of their advantages, disadvantages and applications, and guidance is provided on the  
23 selection of an appropriate modelling approach. Finally, future research challenges are  
24 identified, including system boundary, data uncertainty and modelling, underlying  
25 mechanism of nexus issues and system performance evaluation. This review helps bring  
26 research efforts together to address the challenging questions in the nexus research and  
27 develop sustainable and resilient water, energy and food systems.

28

29 **Highlights:**

30 1. Two definitions of nexus exist but they can be unified under integrated system  
31 assessment

32 2. Nexus research is classified into three questions: internal relationship, external  
33 analysis, system evaluation

34 3. Nexus modelling should consider research questions, system scales and data  
35 availability

36 4. Future research challenges are identified to develop sustainable and resilient nexus  
37 systems

38 **Keywords:** water-energy-food nexus; definitions; research questions; uncertainty;  
39 system evaluation

40

## 41 **1 Introduction**

42 The global demand for water, energy and food is driven by rapid population  
43 increase, urbanization, and climate change and it is estimated to increase by over 50%  
44 by 2050, compared with the 2015 level (Ferroukhi et al., 2015). This will pose a huge  
45 pressure on existing water, energy and food systems, which have already been  
46 constrained due to the competing needs for limited resources in many parts of the world.  
47 More importantly, water, energy and food are interlinked, for example, extreme  
48 droughts caused by climate changes can lead to significant food and energy security  
49 problems due to intensified water supply stress. Under such circumstances, the concept  
50 of water-energy-food nexus was conceived to study and manage the global resource  
51 systems (e.g., water, energy and food) comprehensively (Smajgl et al., 2015; Rasul,  
52 2016; Yillia, 2016).

53 The concept of the ‘nexus’ has gained increasing attention in the research and  
54 policy making communities (Garcia and You, 2016; Weitz et al., 2017). Such  
55 systematic thinking is valuable, as ignorance of the interlinkages among these three  
56 sectors may result in unforeseeable, adverse consequences. Biofuel is one of the vivid  
57 examples. The rapid bioenergy development, which was initially advocated to mitigate  
58 climate change by shifting away from fossil fuels, has the potential to cause biodiversity  
59 loss (Meehan et al., 2010) and food crisis by land use changes, as biomass crops may  
60 compete with food for water and land. Similar cases can also be found in technology  
61 applications where the adoption of water-conserving irrigation and desalination  
62 technologies may create pressures in energy sector through intensive energy  
63 consumptions.

64 Significant efforts have been made to explore the water-energy-food nexus from  
65 various aspects, including calculation of resource flows and their dependencies,  
66 assessment of technology and policy applications, and quantification of system  
67 performance. What’s more, several literature reviews have been published to illustrate  
68 the concepts of water-energy-food nexus (Biggs et al., 2015; de Grenade et al., 2016;  
69 Wichelns, 2017; Cai et al., 2018), simulation tools (Kaddoura and El Khatib, 2017; Dai  
70 et al., 2018), and nexus governance (Weitz et al., 2017) or implementation (Vakilifard  
71 et al., 2018). This helped to improve people's perceptions about the water-energy-food  
72 nexus. However, none of the reviews provides a critical analysis of nexus concepts,  
73 research questions, and their implications on the selection of modelling approaches  
74 (Chang et al., 2016). Hence, in this paper, we provide a critical review on the water-

75 energy-food nexus from three aspects, including the nexus concepts, research questions  
76 and methodologies, and identify the directions and challenges for future research. This  
77 will help bring research efforts together to address the challenging questions in the  
78 nexus and develop the consensus on building sustainable and resilient water, food and  
79 energy systems.

## 80 **2. Research methodology of literature review**

81 With an aim to illustrate the concepts and applications of the water-energy-food  
82 nexus, a database consisted of published articles all over the world from the Web of  
83 Science and Google Scholar was established. Keywords such as “water-energy nexus”,  
84 “water-food nexus”, “water-energy-food nexus”, “climate change & food-energy-water  
85 nexus”, “bioenergy & water”, “water-energy nexus & modelling”, were chosen as  
86 search terms. Special attention had also been paid on the policy related research to  
87 identify applications of nexus in natural resources management. To cover a wide range  
88 of relevant research, we supplemented papers pertaining to environment, resource  
89 recovery, water footprints, energy production, and food consumption patterns. After  
90 that, we exclude irrelevant papers by reading their abstracts and conclusions. The final  
91 sample consisted of 161 documents, ranging from 2002 to 2018.

92 To extract the main focuses in the field of water-energy-food nexus, the selected  
93 papers were read multiple times. Then the major findings of each paper were noted,  
94 together with their research scale, adopted methods, illustration of nexus concepts and  
95 limitations. After that, we held several group meetings to discuss the assessments of  
96 each article as well as the classification method of the selected papers to reach a  
97 consensus on the subsequent analysis. Finally, the selected papers were classified  
98 according to their definitions of nexus, research questions, scales and adopted methods.  
99 Challenges for future research were also identified by summarizing limitations of the  
100 selected papers. Those aspects will be presented in the following sections with more in-  
101 depth analysis.

## 102 **3 Definitions of nexus**

103 The popularity of the nexus could be dated back to the World Economic Forum in  
104 2008, where the global challenges related to economic development were recognized  
105 from the water–energy–food nexus perspective. However, no consensus on the nexus  
106 definitions has been agreed upon (Smajgl et al., 2015; Keskinen et al., 2016; Endo et  
107 al., 2017), with varying interpretations in different sectors, in different contexts and by

108 different researchers (Keskinen et al., 2016). In general, there are two categories of  
109 definitions as below.

110 In the first category, the nexus is interpreted as the interactions among different  
111 subsystems (or sectors) within the nexus system (Sanders and Webber, 2012). For  
112 example, the water-energy nexus can be presented as the interdependencies between  
113 energy and water, as they are coupled in their supply, processing, distribution and use  
114 (Liu et al., 2016). Likewise, when the system boundary is further extended to a water-  
115 energy-food system, the nexus can be defined as the interlink between water, energy  
116 and food (Gulati et al., 2013; Lawford et al., 2013). Thus, water is needed during the  
117 production processes of both energy and food. Energy is required for water abstraction,  
118 distribution and treatment. In contrast, food can also be used to generate energy in the  
119 form of biofuels. Recently, Cai et al. (2018) has further illuminated the interactions  
120 between water, energy and food from three respects, including the interconnected  
121 processes (e.g. physical and chemical), the input-output relations during resource  
122 production, as well as the interactions dominated by institutions, markets, and  
123 infrastructure. In a word, this category focuses on the representation of interactions  
124 between different sectors, aiming at grasping the overall characteristics of the complex  
125 system by its components' interlinkages. As the security issues of these three sectors  
126 become severe, the term emphasizes that failures in one sector may exert pressures on  
127 the other two sectors, requiring a holistic management among these sectors.

128 In the second category, which is more prevalent, the nexus is presented as an  
129 analysis approach to quantify the links between the nexus nodes (i.e., water, energy and  
130 food). There are many interpretations about this emerging approach. For example, the  
131 Food and Agriculture Organization of the United Nations highlighted that the functions  
132 of the nexus approach was to systematically analyze the coupled human-nature system,  
133 and to produce an integrated management of natural resources across different sectors  
134 and scales by building synergies and managing trade-offs (FAO, 2014). While C. A.  
135 Scott et al. (2014) held the view that the essence of nexus was to produce a resource  
136 recovery, with the byproduct of resource use efficiency improvements. Smajgl et al.  
137 (2015) deepened the understanding of this approach to a continuously evolving system,  
138 arguing that the interactions among nexus nodes ought to be dynamically addressed.  
139 Meanwhile, Keskinen et al. (2016) contended that the content of the nexus is so rich  
140 that it could not be interpreted from a single perspective. Therefore, they preferred to

141 define it from three aspects, including an analytical method, governance tool and an  
142 emerging discipline, which complemented one another.

143 Despite the differences between two definitions above, we can conclude that the  
144 nexus is put forward to call for an integrated management of the three sectors by cross-  
145 sector coordination in order to reduce unexpected sectoral trade-offs and promote the  
146 sustainable development of each sector. In this regard, it differs from conventional  
147 decision-making practices that are previously considered within separate disciplines  
148 (Liu et al., 2015).

#### 149 **4 Research questions**

150 The nexus encompasses a broad range of issues and therefore studies on this topic  
151 vary considerably in terms of their focuses. There are many ways to classify current  
152 nexus research questions. For example, as for the number of nodes, current studies  
153 could be divided into three categories, namely, two-node nexus research (e.g., energy-  
154 irrigation (Mukherji, 2007; Shah et al., 2007), energy-water (Marsh and Sharma, 2007;  
155 Hussey and Pittock, 2010; Gheewala et al., 2011; Lu and Thisse, 2011; Stillwell et al.,  
156 2011; Li et al., 2012), food-energy (Walsh et al., 2018), water-land (Chen et al., 2018)),  
157 three-node nexus studies (e.g., water-energy-food (Smidt et al., 2016), energy-food-  
158 water (Howarth and Monasterolo, 2016), water-energy-climate (Mu and Khan, 2009),  
159 land use-climate change-energy (Dale et al., 2011), environment-water-climate  
160 (Groenfeldt, 2010)), and four-node nexus studies (e.g., water-food-energy-climate  
161 (Waughray, 2011; Beck and Walker, 2013), climate-land-energy-water (Hermann et al.,  
162 2012)). If we focus on the framework arrangement of nodes within the nexus, the  
163 current research can be divided into two categories: with a center (Hoff, 2011; Ringler  
164 et al., 2013; Rasul, 2014) and no center (Bizikova et al., 2013; Benson et al., 2015).  
165 Their differences lie in how important each of nexus sectors is compared with others.  
166 In other words, frameworks with certain centers usually emphasize the role of the center  
167 in the entire nexus system, indicating that changes in the framework center dominate  
168 the state of other related sectors through their interlinkages directly.

169 Treating the coupled system as a circle comprised of several subsystems, we  
170 propose to classify the research questions into three categories: internal relationship  
171 analysis, external impact analysis, and evaluation of the coupled system. Such  
172 classification, which focuses more on the connections between different sectors as well  
173 as the descriptions of coupled system performance, is helpful to understand the nexus

174 connotation and extension, as it distinguishes system response to external environment  
 175 (e.g. climate change and policies) from the inner features of the coupled system. This  
 176 also provides valuable insights for decision-makers in policy making and assessment.

177 **4.1 Internal relationship analysis**

178 The internal relationship analysis presents inner features of the coupled system by  
 179 capturing the interactions between different sectors. To make a clear outline of the  
 180 internal relationship analysis, the interactions between different sectors are  
 181 distinguished as one-way impact analysis and interactive impact analysis, as shown in  
 182 Table 1.

183 **Table 1**

184 The internal impact analysis.

	<b>One-way impact analysis</b>	<b>Interactive impact analysis</b>
Connections	♦ Unilateral relationship	♦ Mutual relationships <ul style="list-style-type: none"> <li>▪ Bilateral relationship</li> <li>▪ Feedback loops</li> </ul>
Advantages	<ul style="list-style-type: none"> <li>♦ Lower requirements of resources (e.g. data, time, human, financing)</li> <li>♦ Manifest how changes in one specific sector affect other sectors</li> <li>♦ Facilitate preliminary assessments of trade-offs</li> <li>♦ Serve as a starting point towards integrated managements</li> </ul>	<ul style="list-style-type: none"> <li>♦ Provide more comprehensive assessments of nexus systems</li> <li>♦ Determine the control or dependence role among multiple sectors</li> <li>♦ Identify the driving factors or processes</li> <li>♦ Inspire new solutions for nexus issues from holistic perspectives</li> </ul>
Disadvantages	♦ Manifest limited capacity in nexus analysis due to inability to reflect feedback and second-round effects	♦ Resource intensive in terms of time, data, human and financing
Characteristics	♦ Simple and targeted	♦ Complex and holistic

185

186 The one-way impact analysis, which manifests how changes in one specific sector  
 187 may affect its associated sectors, has the potential to provide valuable preliminary  
 188 insights for decision making even without a comprehensive description of the whole  
 189 nexus system (Ferroukhi et al., 2015), as it accounts for the potential trade-offs between  
 190 different sectors to some extent. Many studies employ this one-way impact analysis to  
 191 investigate nexus impacts due to its analytical simplicity and lower requirements of  
 192 research resources (e.g. data, time, financing, etc.). For example, Babel et al. (2011)  
 193 found that land use change caused by biofuel production may have an adverse impact  
 194 on water quality and quantity, noting that physical and environmental aspects ought to  
 195 be taken into account in bioenergy policy making. Kondolf et al. (2014) investigated

196 the impacts of rapid development of hydropower dams and found that an unprecedented  
197 boom of hydropower dams might result in a greater sediment starvation, leading to a  
198 profound effect on downstream productivity of the Mekong River (Winemiller, 2017).

199 Recently, this one-way impact analysis has been widely employed to analyze the  
200 impacts of applications of new technologies within a certain sector on others, as the  
201 development of new technologies provides new ways to address the scarcity of  
202 resources, with significant impacts on current interlinkages between nexus sectors. To  
203 capture the impact of shifts toward more energy-intensive water use, Sanders and  
204 Webber (2012) made a water-related energy consumption estimation within “energy for  
205 water” system boundaries, indicating that the direct water and steam services account  
206 for 12.6% of the 2010 annual primary energy consumption in the United States.  
207 Likewise, energy consumption in wastewater treatment plants can be reduced under  
208 innovative technologies of energy recovery (Stillwell et al., 2010), integrated real time  
209 control (Meng et al., 2017), and operational permitting (Meng et al., 2016). In contrast,  
210 Denooyer et al. (2016) demonstrated that the cooling technology shift from open-loop  
211 to closed-loop can reduce water withdraws but increase water consumption, noting that  
212 site-specific factors are critical to the choice of thermoelectric cooling technologies as  
213 increase in water consumption may cause unintended consequences downstream.

214 Although above one-way impact studies facilitate preliminary assessments of  
215 nexus impacts and trade-offs, they merely draw a partial picture of nexus systems and  
216 manifest limited capacity in nexus analysis owing to their inability to reflect feedback  
217 and second-round effects (Ferroukhi et al., 2015). Different from the simple unilateral  
218 impact analysis, the interactive impact analysis could describe the characteristics of the  
219 nexus more comprehensively. It can reveal the mutual interrelationship between  
220 different sectors through bilateral relationships and feedback loops, which helps to  
221 determine the control or dependence role among multiple sectors and identify the  
222 driving factors and processes in the development of the coupled system. For example,  
223 setting in the context of transboundary basins, Keskinen et al. (2016) qualitatively  
224 evaluated the bilateral relations between water, energy, and food in major basins of  
225 South Asia and Central Asia, noting that energy and food had greater impacts on water  
226 resources in Central Asia while the impact of water supply changes on food was more  
227 pronounced in South Asia. The results of Siddiqi and Anadon (2011) showed that the  
228 dependence of energy sector on water resources was weak, whereas the dependence of  
229 water abstraction, desalination, and treatment processes on energy was strong in Middle



230 East and North Africa.

231 Besides, numerous studies attempt to present the interactive impacts between  
232 different sectors by depicting their feedback loops through interactions, as changes in  
233 the feedback strength and rearrangement of couplings may characterize the dynamics  
234 of the system (Kumar, 2015). For instance, wastewater reuse for agricultural production  
235 inspired new solutions to advancing the food-energy-water nexus in arid-regions by  
236 reducing energy consumptions required for fertilizer and increasing agricultural yields  
237 in arid-regions with poor soils, as well as improving water quality by nutrient retention  
238 in agriculture irrigation (Mortensen et al., 2016). While Zaman et al. (2012) found that  
239 application of tractor in agricultural production led to more energy demand in Pakistan  
240 which in turn stimulated the increase of its irrigated agricultural land and share of  
241 agriculture value in economy from 1975 to 2010.

#### 242 **4.2 External impact analysis**

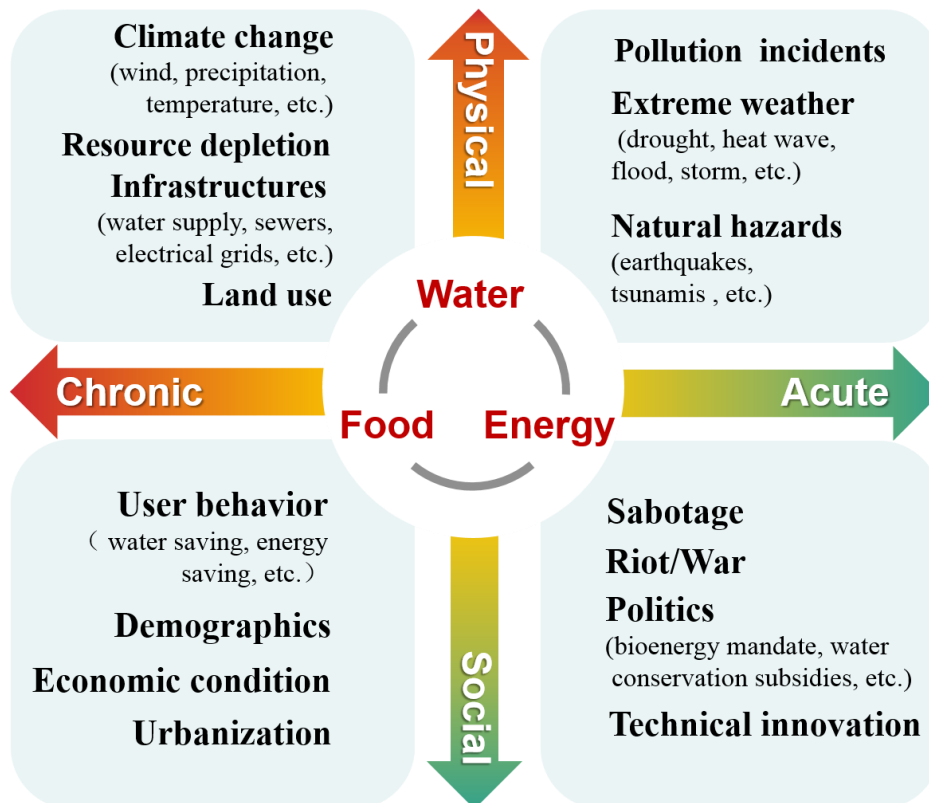
243 The water-energy-food nexus system is usually set in a certain circumstance. Any  
244 external environment changes can complicate the performance of nexus systems by  
245 shaping the production and use of water, energy and food through interconnected  
246 processes. The categorization structure employed by Butler et al.(2017) for external  
247 threats in water systems is extended to water-energy-food nexus systems. Here, external  
248 threats refer to the impacts of outside force, entity, or actor (climate change, pollution  
249 incidents, population growth, politics, etc.). The underlying motivation of partitioning  
250 of external and internal factors (or threats) is to identify key factors that drive nexus  
251 system dynamics. It is also helpful to define system boundary and clarify research issues  
252 at the initial or modelling stage. What's more, partitioning of the driving factors enables  
253 us to conduct a more targeted analysis and provide valuable insights for prioritization  
254 of interventions (Butler et al., 2017), although the categorization is subjective to some  
255 extent.

256 The external impact factors can be classified into four categories based on their  
257 sources and occurrence time, as shown in Fig. 1. According to their sources, external  
258 factors can be classified into two groups, including physical and social causes. Physical  
259 factors such as climate change, extreme weather and natural hazards may change the  
260 provision of water, energy and food by influencing their supply chains and production  
261 processes. Extreme weather such as droughts and floods might have significant  
262 negative impacts on agricultural productivity (Challinor et al., 2010; Bandara and Cai,  
263 2014) and energy generation (Famiglietti, 2014) through water availability. It has been

264 proved that both a hotter climate (with more consumptive water use) and a wetter  
265 climate (with increasing irrigation areas ) could increase the water and energy use for  
266 crops in river basins where agricultural production relies on canal water and  
267 groundwater pumping for irrigation (Yang et al., 2016). Beyond that, higher potential  
268 evaporation caused by climate change may even increase tradeoffs between  
269 hydropower generation and irrigation water use due to decreased water availability  
270 (Zeng et al., 2017). While social factors such as user behavior and perception may move  
271 the focus of resources management from supply side to demand side. For instance,  
272 human dietary habits can change energy use and water footprint throughout the food  
273 supply chain. Shifts from current food consumption patterns in US to a food mix diet  
274 could increase energy use by 38%, and blue-water footprint by 10% (Tom et al., 2016).  
275 In addition, policies and technology may impact the nexus systems through interactions  
276 between different resources. It has been demonstrated that agricultural policies in China  
277 aiming to improve food security and self-sufficiency may lead to a remarkable decline  
278 in local groundwater resources (Ghose, 2014). What's worse, agricultural water  
279 conservation subsidies and applications of more efficient irrigation technologies may  
280 actually aggravate water depletions by reducing valuable return flows and limiting  
281 aquifer recharge (Ward and Pulido-Velazquez, 2008).

282 The external factors can also be divided based on their occurrence time. The  
283 occurrence of extreme weather as well as natural hazards may change nexus systems in  
284 a relatively short time. It has been demonstrated that the hydropower production in the  
285 Iberia was reduced by 40 % due to the 2004/05 drought (García-Herrera et al., 2007).  
286 To survive the drought, the countries in Iberian Peninsula switched to massive imports  
287 of fossil fuel to produce less water-intensive power (García-Herrera et al., 2007),  
288 achieving the decoupling between water and energy sector. Such situation is also suited  
289 to policy changes which may affect human behaviors rapidly. A recent study conducted  
290 by Housh et al. (2015) demonstrated that implementing the mandate for cellulosic  
291 biofuel production (e.g. Miscanthus) on the Mississippi River Basin had the potential  
292 to reduce the nitrate-N loads but introduce stress on streamflow and associated  
293 ecosystem services by increasing the water consumption through Miscanthus  
294 cultivation. However, the period to recognize the impacts of population growth (Mu  
295 and Khan, 2009), climate change (Waughray, 2011; Beck and Walker, 2013) and land  
296 use (Al-Bakri et al., 2013) on nexus systems is much longer. Comparing the conditions  
297 in the year of 2000 to those in 2030 and 2050 respectively, Mu and Khan (2009)

298 indicated that an increasing grain demand caused by population growth may require  
 299 further intensification of land and water use, and climate change might cause declines  
 300 of availability in both surface water and groundwater resources. While [Berardy and](#)  
 301 [Chester \(2017\)](#) found that the temperature increase due to climate change over multiple  
 302 decades is expected to result in more water and energy consumption through increasing  
 303 irrigation requirements in Arizona where agriculture has a high dependency on energy-  
 304 intensive water supply.



305  
 306 **Fig. 1.** The classification of external factors.  
 307

308 Besides the above concerns, the term of nexus is also directed to manage the  
 309 complex nexus system efficiently and sustainably ([Anik Bhaduri and Scheumann,](#)  
 310 [2015](#)). Some researchers have attempted to evaluate the effectiveness of policies from  
 311 diverse interest groups through a nexus prospective. Establishing an energy-water-  
 312 land nexus system, [Howells et al. \(2013\)](#) estimated that the benefits of a local biofuel  
 313 development related policy, which was proposed to guarantee the energy security  
 314 indoor and to reduce GHG emissions, were precarious due to climate change in  
 315 Mauritius. Investigating two possible joint operation modes of Rogun Dam and Nurek  
 316 Dam, [Jalilov et al. \(2016\)](#) suggested that neither the Energy Mode nor the Irrigation  
 317 Mode could lead to optimal benefits for all the riparian countries from the water-

318 energy-food nexus perspective.

### 319 **4.3 Evaluation of the coupled system**

320 Except for internal and external impact analyses, assessment of the whole system  
321 performance, such as resilience (Hosseini et al., 2016) and sustainability (Nguyen et al.,  
322 2014), is another nascent field of current research.

323 Resilience refers to the ability of a system maintain and recover its essential  
324 functions during and after an external shock or disturbance (Hosseini et al., 2016).  
325 Evaluation of resilience of the nexus system is important for comprehensive  
326 management of complex system and rational exploitation and utilization of resources,  
327 as irreversible changes may occur once the external disturbance beyond a certain range.  
328 Attempts have been made to evaluate the system performance under changing  
329 environment from resilience perspective. For instance, Suweis et al. (2015) found that  
330 the resilience of a coupled population-food system was losing due to the increasing  
331 dependency of food security on global trade. The negative impacts of policy changes  
332 on system resilience have also been identified. It was demonstrated that water  
333 conservation (e.g. improvements in irrigation efficiency) subsidies could result in an  
334 increasing water use through irrigation expansion. What's worse, such policy change  
335 may even aggravate water scarcity, deteriorate water quality, and impair river basin  
336 resilience through loss of flexibility and redundancy (C. A. Scott et al., 2014). Beyond  
337 that, the term of resilience is also useful to validate the coping strategies in response to  
338 climate disruption within nexus systems. The study conducted by Scanlon et al. (2013)  
339 suggested that applications of natural gas in power generation were feasible to cope  
340 with water-energy nexus issues along with droughts as they consumed less water in  
341 electricity generation compared to traditional coal or nuclear power plants, which  
342 contributed to the resilience enhancement of power plant during droughts.

343 Besides resilience, system sustainability, which represents system's ability to  
344 continue its functionality with limited resources indefinitely, is also important for  
345 coupled systems, as ignorance of it may result in shortsighted policies which may work  
346 initially but fail in the long run. Establishing a biofuel production system consisting of  
347 three subsystems (e.g. water supply, biomass production and biofuel), Nguyen et al.  
348 (2014) demonstrated that raising the dependencies of water supply on biomass  
349 production may decrease the system sustainability, implying that the quality of the  
350 coupled system may degrade as time went on. However, due to the vague definition of  
351 system sustainability, quantifications of this performance measure are still limited.

## 352 **5 Modelling approaches**

353 There are various methodologies for the nexus research, however, research  
354 priorities, aims, scales and data availability are found critical to decide which approach  
355 should be used for the water-energy-food nexus research. Moreover, no single approach  
356 is applicable for all situations (Endo et al., 2015; Liu et al., 2017).

357 As illustrated in Fig. 2, the appropriate methods vary in response to the scale and  
358 research priorities of a specific nexus system. Specifically, a higher degree of data  
359 aggregation is likely to be required as the system scale moves up. Conversely, more  
360 detail of the inner mechanism of the nexus system, both social and physical should be  
361 represented, as the system scales down. Accordingly, models, such as the computable  
362 general equilibrium model, econometric analysis, and ecological network analysis, play  
363 important roles in large scale nexus research as their consideration of man-made links  
364 (e.g. global supply chains of food and energy (Lawford et al., 2013)) creates  
365 opportunities to investigate the socioeconomic interactions between remote places  
366 (Silviu, 2015). However, the investigation and mathematical methods can be applied to  
367 illustrate nexus issues at almost all scales due to their strength in overcoming data  
368 absence and providing valuable insights during an initial stage. While the agent-based  
369 model is much more suitable for revealing the individuals' decision impacts for their  
370 consideration of individuals' heterogeneities and life-cycle analysis exert its advantages  
371 in assessments of policy and technology shift pertaining to resources consumption and  
372 environment. Besides, the integrated index is powerful to include various social and  
373 environmental factors in policy planning.

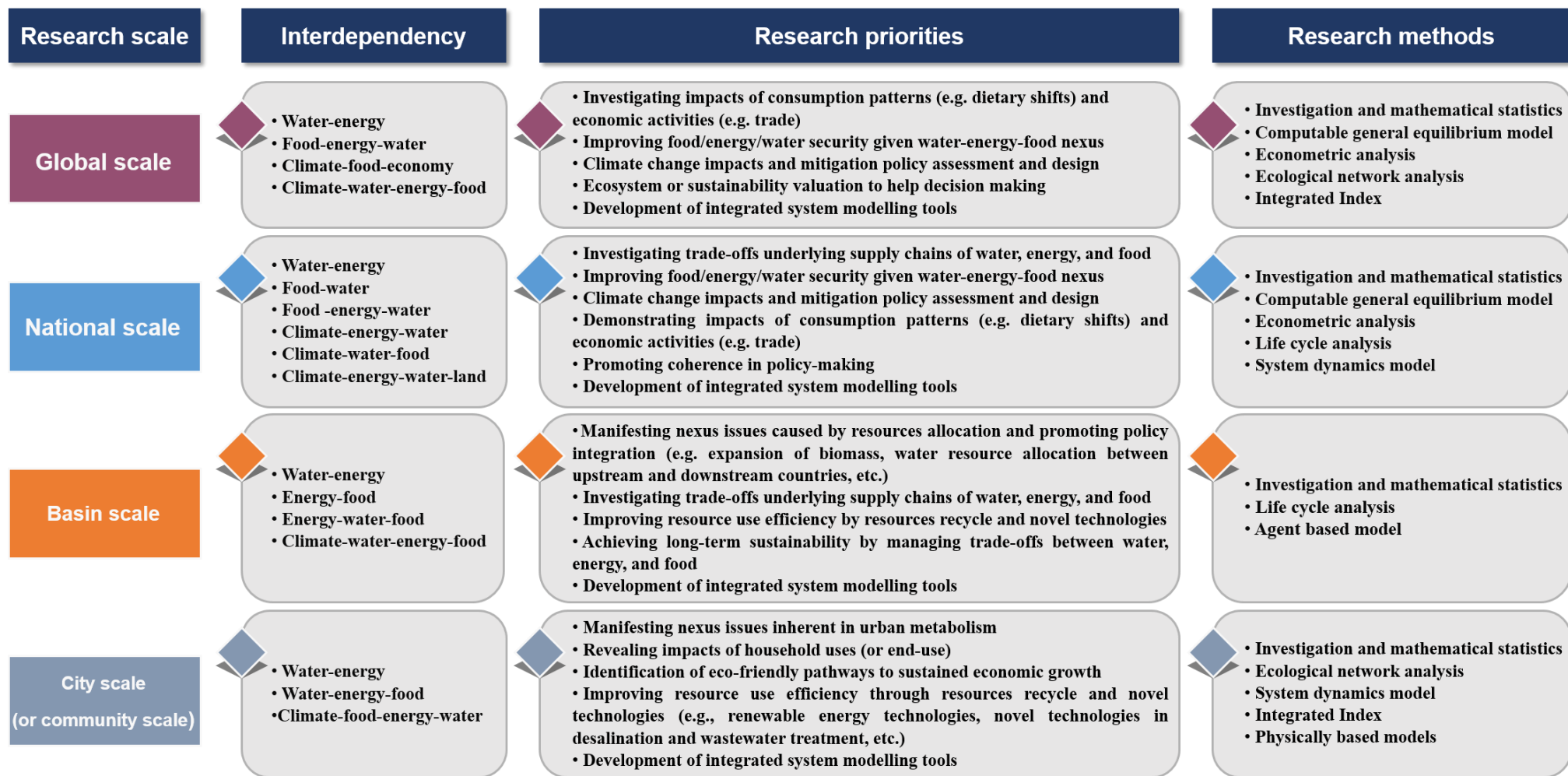


Fig. 2. Summary of nexus research methods and their applications.

374

375

376 Based on the state-of-the-art research methods, the eight key approaches, i.e.,  
377 investigation and statistical methods, computable general equilibrium model,  
378 econometric analysis, ecological network analysis, life cycle analysis, system dynamics  
379 model, agent based modelling and integrated index, are discussed briefly in terms of  
380 their advantages, disadvantages and applications, with an aim to identify research gaps  
381 in current nexus methods.

## 382 **5.1 Investigations and mathematical statistics**

383 Investigations and mathematical statistics, which illustrate nexus issues through  
384 field surveys, expert panel, and collections of public data released by local agencies and  
385 governments, and related literatures, are the most widely used methods to explore the  
386 interactions between nexus sectors . Tracing related resources consumptions associated  
387 with the production process of a certain resources, researchers could make quantitative  
388 assessments about the interactions between water, energy, food and other resources  
389 through data analysis. Adopting such method, [Machell et al. \(2014\)](#) identified that  
390 electric power generation accounted for approximately 15% of total global freshwater  
391 water withdrawals and about 70% of global water was consumed by food production.  
392 While [Ramirez et al. \(2006\)](#) revealed that strong hygiene regulations may account for  
393 one or two-third of the total increase of energy consumption in the meat industry of  
394 four European countries as the temperature of water used for cleaning and sterilization  
395 increased from 60 °C in 1990 to 82 °C in 2001 for the sake of food safety. Through  
396 field surveys, [Alimagham et al. \(2017\)](#) found that conventional scenarios of soybean  
397 production are more environment-friendly in comparison with mechanized scenarios  
398 because of their lower energy consumption and GHG emissions.

399 Such methods are also useful to capture pivotal factors (e.g. climate change, land  
400 use changes, demographics, basin infrastructure) which dominate the evolution  
401 processes of the water-energy-food nexus system. Aggregating the questionnaire  
402 responses across all respondents, [Lawford et al. \(2013\)](#) obtained the ranking of the  
403 importance of different factors that may influence the Water-Energy-Food Nexus, and  
404 provided some recommendations to improve the sustainability of each individual sector  
405 based on the ranking. Likewise, [Smajgl et al. \(2015\)](#) succeeded in formulating the  
406 dynamic framework of water-energy-food nexus in Mekong basin by identification of

407 interlinked variables between different sectors through the Delphi technique which  
408 relied on investigations of a panel of experts.

409 The studies above demonstrate the fact that there exist complex interlinkages  
410 between nexus sectors, and qualitative analyses (e.g., [Lawford et al. \(2013\)](#), [Smajgl et  
411 al. \(2015\)](#)) can bring some valuable insights into decision making. Moreover, key  
412 variables, which can be potentially estimated for a broad range of impact categories at  
413 various scales (global, national and local scales), pave the way for an integrated nexus  
414 modelling and assessment ([Liu et al., 2016](#)). Yet, statistical approaches cannot provide  
415 insights into the internal mechanism of interactions between water, energy and food,  
416 resulting in great difficulties in policy making and evaluating.

### 417 **5.2 Computable general equilibrium model**

418 The computable general equilibrium model (CGE) is a kind of economic model,  
419 which is widely applied to policy analyses pertaining to economy ([Silviu, 2015](#)). The  
420 CGE models can evaluate the impacts of policies on the nexus systems through price  
421 mechanism by grasping the interlinkages relevant to market behavior and changes ([Ge  
422 et al., 2014](#)). Considerable progresses have been made in nexus quantifications with  
423 various CGE models, including GTAP-W model ([Calzadilla et al., 2011](#)), GEM-E3  
424 model ([Kancs and Wohlgemuth, 2008](#); [Németh et al., 2011](#)) and IMPACT model  
425 ([Rosegrant et al., 2002](#)). Using the GTAP-W model, [Calzadilla et al. \(2011\)](#)  
426 demonstrated that the effects of trade liberalization on agricultural production and water  
427 use are modest. While [Wianwiwat and Asafu-Adjaye \(2013\)](#) identified that promoting  
428 bio-liquid policies would increase the price of manufactured food and decrease the food  
429 manufacturing in the short term, but their effects would be smaller in the long run,  
430 indicating that the adverse impacts of such policies on food security were limited in the  
431 long term. Similar research is also conducted by [Ge et al. \(2014\)](#), which shows that  
432 even though the expansion of non-grain fuel ethanol raises the food prices by  
433 intensifying the competition of land, capital and labor between food and fuel ethanol  
434 production, a supply of marginal land to non-grain fuel ethanol can still enhance the  
435 food security in China by reducing food imports, providing valuable insights to manage  
436 the trade-off between biofuel energy production and food security.

437 Although the CGE model could provide a comprehensive interpretation about the  
438 macro-economy and its interaction with the natural resource system, challenges in the  
439 above methods still exist. With a large number of parameters involved, the validity of  
440 the model results highly depends on the quality of the data which are used in model



441 calibration. Moreover, the hypothesis about the economy within the model is somewhat  
442 identical or simple that it may not in accordance with the realities, leading to a large  
443 deviation of the policy evaluation.

### 444 **5.3 Econometric analysis**

445 Econometric analysis employs statistical methods to provide empirical content to  
446 economic relations by analyzing non-experimental economic data (Wooldridge, 2012).  
447 The method of multiple regression analysis lays the foundation for econometric  
448 analysis. However, econometric analysis is different from general statistical methods  
449 introduced in Section 5.1, as it manifests nexus systems through a set of mathematical  
450 equations and elucidates nexus issues based on economic theories.

451 Econometric techniques and procedures have been widely used to infer causality  
452 (Huang et al., 2008) and test economic theories (Pao and Tsai, 2011; Allard et al., 2018)  
453 in the field of nexus research. For example, the regression results of Zaman et al. (2012)  
454 empirically revealed the bi-directional causality between agricultural growth and  
455 energy consumption in Pakistan, demonstrating that actions pertaining to promoting  
456 energy efficiency and diversifying energy sources will indeed contribute to sustained  
457 economic growth in Pakistan where agriculture plays a dominant role in economy. Pao  
458 and Tsai (2011) confirmed the Environmental Kuznets Curve hypothesis for the four  
459 BRIC countries, noting that the relationship between CO<sub>2</sub> emissions and gross domestic  
460 product fits an inverted-U curve.

461 Beyond the above research, numerous attempts have also been made to examine  
462 the validity of existing policies. A recent research, which investigated the impacts of  
463 biofuel production on the ecosystem in six regions of the world through panel  
464 econometric techniques, confirmed the conclusion that expansion of biofuels was not a  
465 good choice to cope with climate change given its negative impacts on biodiversity and  
466 water resource at the global scale (Zaman et al., 2016). Similar methods have been  
467 utilized to provide recommendations for future policy design. Ozturk (2015) manifested  
468 the food-energy-water nexus for the BRICS countries by simultaneously modelling  
469 each individual sector that was linked separately to multiple regressors, noting that food  
470 security may be challenging for the five countries as the demand and supply gaps of  
471 energy and water widened. This indicates that economic-environmental policies are  
472 imperative to stimulate sustainable development for the BRICS countries in the long-  
473 run, as increasing energy demand for economic growth may lead to environment  
474 degradation among the five countries (Ozturk, 2015).

475 Econometric analysis is more targeted and efficient in policy assessment and  
476 design than general statistical methods. However, analogous to CGE models,  
477 econometric models heavily rely on data (Semertzidis, 2015), and some underlying  
478 assumptions may not be justified (Hamiche et al., 2016). What's worse, misleading  
479 conclusions may be drawn due to ignorance of key variables in econometric models  
480 and application of small data samples (Pao and Tsai, 2011). To get more reliable results,  
481 it is suggested to use large sample sizes, panel data approach (Huang et al., 2008), and  
482 multivariate models to conduct econometric analysis (Zachariadis, 2007; Ozturk, 2010).  
483 In addition, unrecorded economy should be considered to get closer to real economy  
484 when making assumptions in econometric modelling (Ozturk, 2010).

#### 485 **5.4 Ecological network analysis**

486 Ecological network analysis (ENA) evolved from input-output analysis (Chen and  
487 Chen, 2015) is currently one of the main methods for evaluating the interactions  
488 between economic and natural components. Taking systems as the integration of  
489 multiple entities connected by metabolic flows, ENA can offer a unified analysis for  
490 both direct and indirect flows embodied in interwoven chains of production and  
491 consumption, indicating the potential to investigate the trade-off between multiple  
492 elements (Chen and Chen, 2016). It has been used to dissect metabolic flows (e.g. water,  
493 energy, carbon emissions) in urban metabolism (Chen and Chen, 2016; Chen and Chen,  
494 2017a) and global trade of energy (Duan and Chen, 2017) and virtual water (Yang et  
495 al., 2012). Combined with other metrics such as linkage analysis (Lenzen, 2003; Fang  
496 and Chen, 2017), Finn's cycling index (Finn, 1976) and system robustness (Fath, 2015),  
497 ENA is capable to detect the role transition of a sector and quantify the system  
498 performance (cycling and resilience). For example, using Beijing as an example, Chen  
499 and Chen (2016) identified that most urban sectors rely on manufacturing in the energy–  
500 water nexus, and the impact of nexus on energy networks ( $\pm 200\%$ ) is larger than water  
501 networks ( $\pm 30\%$ ). Furthermore, the average robustness of the energy-water nexus  
502 network seemed to be lower compared to natural ecosystems, as it had more intensive  
503 material exchanges (Chen and Chen, 2016).

504 In addition, compartment-oriented ENA metrics such as control allocation and  
505 dependence allocation can identify the control or dependence role among multiple  
506 sectors (or components) by tracking the metabolic (or material) flows (Chen and Chen,  
507 2015). This analysis is critical for locating the driving factors of changing nexus  
508 systems and inspiring new solutions for resources management from both systemic and

509 sectoral levels (Chen and Chen, 2016). For instance, with the aid of control allocation  
510 and dependence allocation, Chen and Chen (2017b) revealed that high-pollution  
511 industries which were moved outside the urban boundary of Beijing, were expected to  
512 have impacts on the local carbon emissions for the constant demand of urban citizens,  
513 indicating that carbon-cutting policies might not be effective unless a full optimization  
514 of supply chains was given. Duan and Chen (2017) applied a similar approach to  
515 investigate the mutual interactions between water and energy inherent in global energy  
516 trade and took China as an example to demonstrate the usefulness of such analysis in  
517 policy design. Their results showed that although no country was controlled by China  
518 via energy trade, the international trade of energy made China's water security more  
519 vulnerable to other countries due to strong water import dependence associated with  
520 energy products. This informed the policy makers that strategies pertaining to reduce  
521 the proportion of water-intensive products in energy import mix are more beneficial.

522 Despite the strength of ENA in analysis of complex interactions, ENA is  
523 essentially a static method due to its steady-state assumption that the inputs must equal  
524 the outputs for each component and the whole network. Hence, the dynamic  
525 characteristics of the network system cannot be captured unless a longitudinal study is  
526 conducted (Yang et al., 2012). In addition, the implication of ENA in urban planning is  
527 still limited due to its sectoral level analysis and the lack of indicators directly related  
528 to land-use based urban planning (Chen and Chen, 2015), although ENA can be related  
529 to environmentally friendly planning for its consumption-based insights (Chen et al.,  
530 2014).

### 531 **5.5 Life-cycle analysis**

532 Life-cycle analysis (LCA) is one of the most widely used methods for quantifying  
533 the environmental impacts of a given product or process throughout its entire life cycle.  
534 It can accurately show the quantification of any unit during its life cycle and easily  
535 export its calculation processes, with the characteristics of identifying all of the inputs  
536 or outputs that may have significant impacts on environment (Nair et al., 2014). Due to  
537 above advantages, LCA approach, which could provide a consistent analytical  
538 framework and environmental data support for decision-making, has been extensively  
539 applied in assessing the environmental impact of nexus sectors across their production  
540 and consumption processes, aiming to seek effective ways to cope with current  
541 resources shortage and global climate change.

542 Using the integrated life cycle assessment (LCA) method, Al-Ansari et al. (2015)

543 made an integrated environmental evaluation of energy, water and food supply chains,  
544 and indicated that food system had the most significant impact on global warming.  
545 While [Feng et al. \(2014\)](#) proved that wind power production, compared to other  
546 electricity generation technologies, would significantly reduce the carbon emissions  
547 and water consumption over its whole life cycle. In addition, LCA has also been  
548 frequently applied for evaluating the impacts of construction and operation of urban  
549 water supply facilities on environment ([Lundie et al., 2004](#); [Friedrich et al., 2007](#); [Foley  
550 et al., 2010](#)). [Foley et al. \(2010\)](#), for instance, demonstrated that operational energy and  
551 greenhouse gas emissions presented a positive relationship with nitrogen removal and  
552 a non-significant correlativity with phosphorus removal in wastewater treatment plants.  
553 Such method is also useful for policy-making by comparing the impacts resulting from  
554 different options. For example, results of [Chang et al. \(2015\)](#) implied that a coal-to-  
555 shale gas shift in power generation was a promising way to a lower water intensive  
556 electricity in China, as the water consumption of shale gas-fired electricity was less  
557 than that of China's present coal-fired electricity given the extraction-to-wire effects.

558 However, the LCA method still has some drawbacks despite its extensive  
559 applications in nexus research. With a high dependency on data, the LCA method is  
560 difficult to apply in data-scarce regions ([Hamiche et al., 2016](#)). Moreover, due to the  
561 subjective decision of the definition about the system boundaries, it is therefore  
562 inevitable to leave out some production processes, which often leads to significant  
563 truncation errors in the calculations of LCA. Further, the LCA seems to be a static  
564 method and may not be directly suitable for dynamic analyses of complex systems ([Nair  
565 et al., 2014](#)). To some extent, it is difficult to consider social factors within a coupled  
566 system based on LCA method with a focus on assessments of environmental impacts  
567 ([Balkema et al., 2002](#)).

## 568 **5.6 System dynamics model**

569 System dynamics modelling (SDM), a top-down modelling method based on  
570 causal mechanism, follows the assumption that system behaviors are determined by  
571 their structures. It allows comprehensive analysis of multi-sectoral systems at both  
572 macro and micro levels by establishing causal feedback loops among the elements  
573 within a certain system. This makes it well suited for multidisciplinary and multi-actor  
574 problems ([Stave, 2003](#)). For example, [Chhipi-Shrestha et al. \(2017\)](#) had adopted such  
575 method to identify critical factors that constrained the sustainability of the urban water  
576 system in Penticton, noting that it was the hot water use that contributed the most to

577 energy use and carbon emissions of the operational phase of the urban water system.  
578 Such approach has also been extensively applied in policy evaluation. Establishing  
579 main causal-loop diagrams of the climate-energy-water nexus, [Newell et al. \(2011\)](#)  
580 found that technology innovation, increase of redundancy in distribution and  
581 transmission networks and a dynamic system thinking in policy-making were helpful  
582 to improve the resilience of the national electricity market in Australia. While [K. El-  
583 Gafy \(2014\)](#) demonstrated that raising the self- sufficiency from wheat in Egypt through  
584 wheat trade pattern policies were expected to increase its wheat cultivated area as well  
585 as water footprint of wheat production for the interval 2010-2050, compared with the  
586 base line scenario in 2010.

587 Such models contribute a lot to overcoming difficulties that may otherwise impede  
588 the development of holistic policies ([Newell et al., 2005](#)). The causal feedback loops  
589 developed by system dynamics model could assist in the identification of the sources  
590 of problem behaviors and the understanding of the feedback structure of the system.  
591 Based on the dynamic analysis under different scenarios, the system dynamics model  
592 could offer optimal system structures to coordinate the various factors within the system  
593 and provide scientific basis for decision-making. However, due to the subjective  
594 abstraction and simplification of the nexus system during modelling process, it is  
595 necessary to involve relevant stakeholders in the SDM modelling process as much as  
596 possible to avoid the inconsistencies between reality and the model caused by subjective  
597 factors.

### 598 **5.7 Agent based modelling**

599 Agent based modelling (ABM) is a “bottom-up” approach where every agent is a  
600 discrete autonomous entity with distinct goals and actions within a particular social  
601 context. By modelling agents individually, the full effects of the diversity that exists  
602 among agents in their attributes and the behaviors can be observed at the bottom level  
603 ([Macal and North, 2010](#)). What’s more, the emergent phenomena at the system level  
604 can also be investigated through aggregation of all agents’ behaviors ([Du et al., 2017](#)).  
605 Thus, agent based modelling breaks through the limitations of single-level and  
606 individual-perspective, and provides a more realistic and effective modelling  
607 framework for describing and investigating complex systems by offering a way to  
608 model social systems that are composed of numerous agents which can interact with  
609 and influence each other, learn from their experiences, and adapt their behaviors so they  
610 are better suited to their environment.

611 Recently, [Ng et al. \(2011\)](#) established an agent-based hydrologic-agronomic  
612 model to explore the interlinkages between the farmers' planting decisions and their  
613 associated effects on stream nitrate load when carbon allowance trading, and markets  
614 for crops (including biofuel crop) are considered. Their results proved the usefulness of  
615 such models for coupled human-environment nexus within a watershed. Hereafter,  
616 [Khan et al. \(2017\)](#) investigated the impacts of agents' water resource management  
617 decisions on the water-food-energy-environment nexus system at watershed scale  
618 through a more generalized ABM framework by coupling the water system model with  
619 SWAT model, noting that the impact of agent preferences on crop production was more  
620 significant than that of hydropower generation. However, due to higher requirements of  
621 data, challenges of noneconomic behaviors' definitions and computational  
622 requirements, application of this method to nexus related issues is currently limited, but  
623 promising in further research.

## 624 **5.8 Integrated Index**

625 The integrated index method usually presents various social and environmental  
626 characteristics of systems by multiple indicators. With the aid of these indicators,  
627 researchers are able to capture the overall properties of nexus systems regardless their  
628 complexity ([Endo et al., 2015](#)). What's more, index based methods contribute a lot to  
629 comparative assessment and benchmarking ([Yigitcanlar et al., 2015](#)) by describing  
630 system performance in a uniform and standardized format. For example, [Kourtit et al.](#)  
631 [\(2017\)](#) derived a holistic picture of sustainability of 39 global cities based on their  
632 efficiency performance indicators, indicating that European cities gain higher  
633 sustainability efficiency scores in terms of their human environment. Beyond that, this  
634 method can also provide valuable information for policy planning by manifesting a  
635 comprehensive outline of nexus issues ([Flörke et al., 2018](#); [Schlör et al., 2018](#)). Taking  
636 urban surface-water deficit as an indicator, [Flörke et al. \(2018\)](#) identified that climate  
637 change and population growth could intensify the competition of water between urban  
638 and agricultural sectors, noting that improvement in irrigation efficiency became an  
639 essential adaptation option to enhance urban water security.

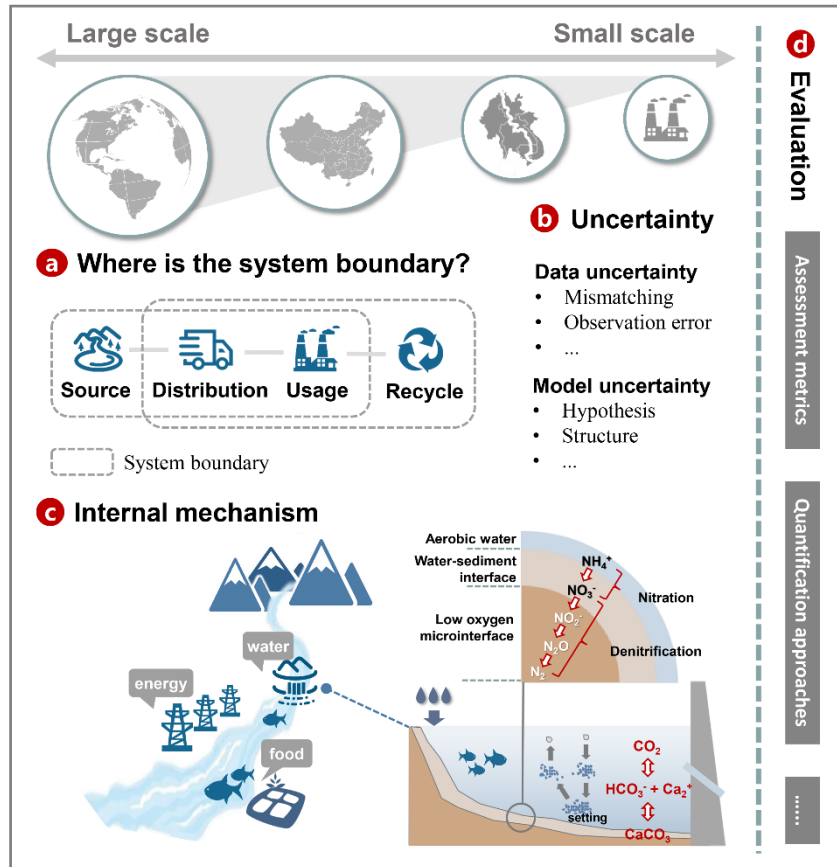
640 As cities become the center of water-energy-food nexus discussion ([Duić et al.,](#)  
641 [2014](#); [Wang and Chen, 2016](#); [Brandoni and Bošnjaković, 2017](#); [Schlör et al., 2018](#)),  
642 efficient managements of nexus systems call for consideration of multidimensional  
643 performance (sociology, ecology, economy, etc.). More integrated indicators should be  
644 introduced to measure the performance of nexus systems in a holistic way ([Yigitcanlar](#)

645 [et al., 2015](#); [Schlör et al., 2018](#)). The UN-Habitat City Prosperity Index (CPI) was  
646 therefore proposed to identify factors that make urban cities become more prosperous  
647 and the areas where policy intervention is needed from five aspects (productivity,  
648 infrastructure, quality of life, equity, and environmental sustainability) ([UN-Habitat,](#)  
649 [2013](#)). After that, attempts have been made to combine CPI with regulations of urban  
650 nexus. [Yigitcanlar et al. \(2015\)](#) proposed a multi-scalar approach to assess the  
651 environmental sustainability of CPI in urban cities and applied it to the Gold Coast to  
652 demonstrate its usefulness. [Schlör et al. \(2018\)](#) established the Nexus City Index (NXI)  
653 based on CPI and employed it to quantify the resilience of the food-energy-water nexus  
654 in urban cities. Their results suggested that NXI put city resilience on a comparable scale  
655 without reducing the complexity of nexus systems and offered opportunities to cope  
656 with prosperity gaps in urban planning ([Schlör et al., 2018](#)). Despite the above  
657 advantages, the application of such indicators in urban planning is still challenging, as  
658 it highly depends on systematic database ([Schlör et al., 2018](#)). In addition, major  
659 difficulties also lie in how to build a rational index system and eliminate the bias  
660 resulting from the use of weights among indicators ([Yigitcanlar et al., 2015](#)).

## 661 **6 Directions of future research and prospects**

662 The existing studies offer a promising outlook for water-energy-food nexus from  
663 different aspects, which can support in assessing trade-offs, predicting potential  
664 (unintended) effects, providing a co-optimization base for different stakeholders who  
665 often have conflicting interests and visualizing the impacts for informed decision  
666 making ([Agboola and Braimoh, 2009](#); [Hurford and Harou, 2014](#); [Santhosh et al., 2014](#);  
667 [Liu et al., 2015](#)). However, limitations of current studies still exist. Grouping the above  
668 analysis together, future directions of nexus research are identified from four aspects,  
669 including the system boundary, data uncertainty and modelling, nexus mechanism and  
670 system evaluation, as shown in Fig. 3.

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### 6.1 System boundary

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**Fig. 3.** Summary of future nexus research directions. (a) Definitions of the system boundary; (b) Date uncertainty and modeling; (c) The underlying mechanism referring to the physical, chemical processes associated with resource flows as well as their supply chains. For example, setting the nexus issue within a water-hydropower-agriculture system, the internal mechanism refers to flow states (e.g. velocity, temperature), sediment transport, growth of algae and biochemical reactions (e.g. nitration and denitrification via the water-sediment interface) along with hydropower generation and food production, as well as decision making mechanisms; (d) The evaluation of coupled nexus system, including assessment metrics and quantitative assessment approaches.

It is of great importance to define the system boundary when conducting nexus analysis, as different system boundary definitions result in different results. For example, [Liu et al. \(2016\)](#) concluded that energy embedded in agricultural, municipal and industrial water use (e.g. irrigation, wastewater collection) accounted for 1.0%–1.9% of total primary energy in the United States in 2010, however, considering a wider range of processes where energy is applied to water for other outputs (e.g. steam-driven power generation), the proportion increased to 47% ([Sanders and Webber, 2012](#)).

The difficulty of system boundary definition lies in how to choose an appropriate



691 boundary. On one hand, a narrow boundary might leave out some important  
692 interlinkages, which means that the description of the nexus system is under-  
693 representation. For example, merely focusing on conflicts between hydropower  
694 generation and irrigation issues with an ignorance of the interactions between water and  
695 inland fisheries in food security may lead to a partial evaluation of water-energy-food  
696 security nexus in riparian countries (Cooke et al., 2016). On the other hand, with a large  
697 system boundary, more processes are included in the nexus system and thus more data,  
698 assumptions and detailed understanding of the processes are required to develop a  
699 nexus model (Garcia and You, 2016). For example, for a global water-energy nexus, a  
700 large number of end-use processes (e.g., dish cleaning) need to be accounted for,  
701 increasing the difficulty of modelling due to varied users (Yillia, 2016) and end-use  
702 processes representation (Kyle et al., 2016). Moreover, it is much more difficult to  
703 extract and synthesize valuable information from different sectors considering their  
704 interactions, as the nexus boundary varies from resource management units to  
705 administrative boundaries (Liu et al., 2017). An appropriate selection of system  
706 boundary is critical for the nexus and thus required for further research.

707 Currently, it has been widely accepted that the definition of system boundaries  
708 should base on research aims (Avellán et al., 2017; Chen and Chen, 2017a; Albrecht et  
709 al., 2018) and data availability (Chen and Chen, 2017a). It is of great importance to note  
710 that water-energy-food nexus can go beyond its system boundaries (Avellán et al., 2017;  
711 Chen and Chen, 2017a). Taking the urban nexus research in Beijing as an example,  
712 Chen and Chen (2017a) suggested that upstream activities (e.g., indirect energy or water  
713 use outside Beijing) beyond the system boundaries ought to be considered due to their  
714 significant impacts on urban metabolism. In this regard, introducing the Driver-  
715 Pressure-State-Impact-Response (DPSIR) framework designed for adaptive  
716 management of Social-Ecological Systems (Gari et al., 2015) into modelling might be  
717 an effective way to demarcate system boundaries, as the scale of the two DPSIR  
718 elements (State Change and Impact) within the system of concern can provide valuable  
719 information for the establishment of system boundaries (Atkins et al., 2011). This has  
720 been demonstrated by Atkins et al. (2011) which showed that DPSIR was capable to  
721 quantify the environmental state changes as well as their impacts on societal benefits  
722 resulting from the pressures.

## 723 **6.2 Data and modelling uncertainty**

724 The themes of the research vary as the research scale changes, as shown in Fig. 2.

725 In the literature, global scale research focuses more on the impacts of climate changes  
726 on agriculture and water availability, as well as the changes in virtual water/ water  
727 footprints caused by the global trade (Yang et al., 2012; Duan and Chen, 2017). At the  
728 national scale, more attention is paid to resource security relevant issues as well as their  
729 associated environment impacts under various policies. While studies pertaining to  
730 quantification of the interactions between water, energy and food at household scale are  
731 more concerned about behavioral and technological factors (Abdallah and Rosenberg,  
732 2014). Different research problems have different data requirements. The larger the  
733 system scale is, the more concerns about social and economic data. However, the data  
734 from government reports and published data are of varying quality and availability  
735 (Perrone et al., 2011), as they are released by different sectors for various purposes  
736 without consistent reporting standards (Ernst and Preston, 2017). The use of these data  
737 may cause great uncertainty in the nexus research. Moreover, some data are aggregated  
738 at large scale (Perrone et al., 2011), making it unsuitable for small scale research. This  
739 is the case in climate-related nexus studies (Vaughray, 2011; Beck and Walker, 2013;  
740 Berardy and Chester, 2017), where application of climate models and their downscaling  
741 (Howells et al., 2013) introduces uncertainty to the final results.

742 What's more, assumptions and simplifications are frequently introduced in nexus  
743 research to deal with data scarcity. For example, Liu et al. (2016) had to assign constant  
744 energy intensity values to water-related processes except desalination in temporal  
745 variability analysis of water-related energy consumption due to lack of data on those  
746 processes. Owing to the lack of empirical data, two extremes of behavior (e.g. cautious  
747 and bold) are defined by Ng et al. (2011) to represent the farmers' behaviors in their  
748 water-energy nexus system through an ABM framework, which means the simulate  
749 results may not adequately represent the reality. Likewise, Jalilov et al. (2016) had to  
750 exclude the groundwater use for irrigation and introduce many assumptions on cropped  
751 area and crop water use in an agronomic model when conducting the water-energy-food  
752 nexus research. Such assumptions or simplifications may help overcome some data  
753 scarcity, however, they can also exert an impact on the final results and even  
754 misrepresent the interactions among nexus sectors. In addition, models such as CGE,  
755 which consist of several sectors including economy, water, crop and energy, may have  
756 numerous sources of uncertainty, ranging from model inputs and structures to scenario  
757 assumptions.

758 To address above issues, endeavors should be made to improve data availability

759 for nexus research. On one hand, special efforts should be made in data monitoring and  
760 collection, data processing as well as uncertainty analysis. Recently, implications of  
761 innovative sensor technologies (Abegaz et al., 2018) (including remote sensing  
762 (Scanlon et al., 2017)) have been demonstrated to have remarkable utility in providing  
763 new data sources. Besides, advanced data science techniques (e.g., machine learning,  
764 correlation analysis, cloud computing (McCabe et al., 2017), Geographic Information  
765 Systems (Cai et al., 2018), etc.) as well as high performance computers are expected to  
766 speed up data uptake and facilitate analysis of massive datasets. Combination of these  
767 techniques indicates a promising future for data uptake and analysis. On the other hand,  
768 there is an urgent need to advance data-sharing through development of new data  
769 sharing mechanism which can stimulate broad participation and cooperation from  
770 different governments, research institutions and communities (Fekete et al., 2015).  
771 Connecting existing and new datasets can produce more accessible and useful data to  
772 prioritize problems, support nexus modelling and inform decisions (DOE, 2014). In  
773 addition, further research on the trade-offs between simplicity and comprehensiveness  
774 in the modelling process will provide new insights to develop appropriate models,  
775 generating robust results with limited data (Kaddoura and El Khatib, 2017). Beyond  
776 that, modelers should make the structure of nexus models more standardized and  
777 modularized, offering opportunities to analyze structural uncertainties better by  
778 exchange and recombination of model components (DOE, 2014).

### 779 **6.3 The underlying mechanism of nexus**

780 Future research needs to characterize the interlinkages between nexus sectors, with  
781 a focus on understanding of the underlying mechanism of the nexus. One of the most  
782 critical knowledge gap is that the majority of current studies focus more on the supply  
783 chains and resource use efficiencies of nexus sectors under different scenarios, for  
784 example, water use in food production (Siebert et al., 2010; Finley and Seiber, 2014),  
785 energy implications in water use (Kahrl and Roland-Holst, 2008). Yet, consideration of  
786 physical, biophysical and chemical processes is important for conceptualizing  
787 relationships of nexus sectors (de Grenade et al., 2016). Knowledge gaps also exist in  
788 interactions between ecological, economic, and social dimensions (Räsänen et al.,  
789 2015).

790 Dynamic quantification methods are required to capture the vital factors affecting  
791 the coupled nexus system performance and to reveal the dynamics of natural processes  
792 along with social processes that underpin the interactions between nexus sectors. For

793 instance, few studies have been conducted to understand how the development of  
794 hydropower will affect soil erosion, sediment transport and nutrient composition (e.g.  
795 the nitrification and denitrification via the water-sediment interface) within rivers. This is  
796 important to identify the systemic risk of runoff utilization, develop adaptive utilization  
797 strategies considering the nexus and evaluate the reasonable exploitation scope of  
798 hydropower.

799 Based on above, there is an urgent need to develop nexus-specific models to  
800 provide a better representation of nexus systems (Albrecht et al., 2018), as implications  
801 of existing models derived from other fields (e.g., LCA from management science and  
802 econometric analysis come from economics) may lead to a partial description of  
803 feedback and interactions of nexus systems due to these models' specific design  
804 purposes (Miralles-Wilhelm, 2016). As nexus elements being considered continue to  
805 expand (Dai et al., 2018), a nexus-specific model ought to be flexible enough to support  
806 module extensions (Chang et al., 2016), reveal physical and social dynamics, and  
807 facilitate analysis across multiple temporal and spatial scales (Albrecht et al., 2018).  
808 Given current data availability, such models are also required to have the ability to  
809 combine quantitative with qualitative data (Albrecht et al., 2018) to alleviate intensive  
810 and extensive data requirements during modelling. In addition, to establish an  
811 integrated and flexible model for water-energy-food nexus, multiple stakeholders and  
812 decision makers should be engaged into modelling processes to incorporate valuable  
813 and timely information from different sectors (e.g., technological descriptions, human  
814 activities) and avoid ignorance of vital processes or interactions owing to the site-  
815 specific nature of nexus (Keairns et al., 2016; Albrecht et al., 2018), which can be done  
816 through better interagency collaborations.

#### 817 **6.4 The evaluation of coupled nexus systems**

818 One motivation of the nexus research is to better manage the water-energy-food  
819 system in order to promote sustainable development under changing environments.  
820 Assessments of the resilience and sustainability of the coupled systems are therefore  
821 important to understand their long-term performance under changing environments.  
822 However, in water-energy-food system, resilience and sustainability depend not only  
823 on the characteristics of the individual subsystems but also on the interlinkages among  
824 different subsystems (Hosseini et al., 2016), as changes in one subsystem may cascade  
825 quickly and widely through the couple system, triggering a series of chain reactions.  
826 The assessment metrics and approaches designed for individual systems may be no

827 longer applicable to the nexus system as a whole. In addition, due to the loose coupling  
828 of nexus sectors in most of current methods (Yillia, 2016), the feedback is usually  
829 considered exogenously, resulting in an inadequate representation of the nexus system.  
830 All these create great challenges for the evaluation of resilience and sustainability of  
831 coupled systems.

832 Thus, efforts are required to investigate the resilience as well as sustainability of  
833 the coupled system, including assessment metrics and quantitative assessment  
834 approaches for nexus systems. However, this might be challenging, as multiple  
835 dimensions (sociology, ecology, economy, etc.) ought to be included to assess nexus  
836 system performance owing to the wide connotation of nexus. Fortunately, emerging  
837 concepts like NXI (Schlör et al., 2018), CPI (UN-Habitat, 2013) and entropy theory  
838 (Tamvakis and Xenidis, 2013) are expected to rectify this situation, as they exemplify  
839 how to combine different aspects of the research system in a holistic way. What's more,  
840 Tamvakis and Xenidis (2013) evidenced that the framework based on entropy theory  
841 was useful to quantify system properties due to their strength in capturing underlying  
842 interactions (including feedback (Mayer et al., 2014)) among system components (both  
843 living and non-living). This study also informed us that transforming system  
844 performance into entropy can facilitate a direct and explicit way for assessing the  
845 overall system behaviors (e.g., resilience (Tamvakis and Xenidis, 2013), sustainability  
846 (Mayer et al., 2014)) through aggregation of behaviors at the component level as a  
847 single metric. This can inspire researchers to use innovative ways in development of  
848 assessment metrics and methods for nexus systems.

## 849 **7 Conclusions**

850 This paper provides a critical review on the concepts, research questions and  
851 methodologies in the field of water-energy-food nexus. The key findings are  
852 summarized below:

853 1) Two definitions of nexus currently exist in literatures, but they can be unified  
854 under integrated system assessment. The first one defines nexus as the interlinkage  
855 between different resources, while the other one treats nexus as a novel approach to  
856 investigate nexus systems with various meanings in different contexts. The two  
857 definitions could be unified through integrated management of the nexus to reduce  
858 unexpected impacts and sectoral trade-offs and promote the sustainability and resilience  
859 of the entire nexus system.

860 2) Current research can be classified into three categories: internal relationship

861 analysis, external impact analysis, and evaluation of the coupled system. Such  
862 classification is helpful to catch the hotspots in nexus studies scattered in various  
863 disciplines, as it stimulates more focuses on the connections between different sectors  
864 as well as the coupled system performance. What's more, partitioning of internal and  
865 external factors enables us to clarify site-specific nexus issues, conduct a more targeted  
866 analysis, and provide valuable insights for prioritization of interventions.

867 3) Eight modelling approaches are discussed in terms of their advantages,  
868 disadvantages and applications, providing guidance on model selection in the nexus  
869 research. It is identified that the connotation of nexus is so rich that no single approach  
870 is applicable in all situations however the appropriate method should be selected  
871 considering research questions, research aims, scales and data availability of the nexus  
872 system changes. For example, the CGE Model is more appropriate to investigate macro-  
873 economy and environmental change at regional and global scales due to its  
874 consideration of man-made links. While ABM is much more suitable for revealing the  
875 individuals' decision impacts for its description of individuals' heterogeneities and  
876 decision-making processes.

877 4) Despite the progress in water-energy-food nexus, limitations of current studies  
878 still exist, and four challenges for future research are identified. Analysis indicates that  
879 current research does not adequately address problems inherent in system boundary  
880 definition as well as the uncertainties associated with data and modelling. What's more,  
881 the internal mechanism analysis of nexus issues is somewhat constrained due to partial  
882 description of nexus systems. Challenges also exist in the evaluation of system  
883 performance, where nexus-specific assessment metrics and quantitative approaches  
884 need to be developed.

885 Therefore, more efforts are required to advance holistic assessments of water-  
886 energy-food nexus. Current discussions suggest that implications of DPSIR framework  
887 in nexus modelling may be useful for clarifying system boundaries, while improvement  
888 in data availability through innovative technologies is promising to address  
889 uncertainties associated with data and modelling. Besides, there is an urgent need to  
890 develop nexus-specific models to elucidate the underlying mechanism inherent in  
891 water-energy-food nexus. Emerging concepts like NXI, CPI and entropy theory are  
892 expected to stimulate more holistic assessments of system performance. These efforts  
893 may also be helpful in providing concise information to support decision-making in  
894 reality. In this regard, this review helps bring research efforts together to address the

895 challenging questions in the nexus research and develop resilient water, energy and  
896 food systems.

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