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System Modelling and Safety Risk Assessment for Region-Wide CCUS Systems

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Carbon capture, utilization, and sequestration (CCUS) is an important option for meeting national carbon neutrality targets. However, the application of CCUS on an industrial scale and the extension of supply chain networks inevitably increase the exchange of information and material flows, creating a "media shifting" from environmental to safety risk issues. This work proposed system modeling and safety risk assessment for integrated regional CCUS systems. Considering CCUS modules, Aspen Plus simulation-based regional CCUS system is constructed. An integrated inherent safety index system is proposed to evaluate the risk characteristics. A CCUS system in Shandong Province is illustrated as a case study to analyze its safety risk. The results show that in terms of the overall inherent safety index, the emission source module has the highest risk, which is 2.67 times higher than that of the biological/geological utilization module.

1. Introduction

Emissions of greenhouse gases exacerbate climate change on Earth. If no effective measures are taken, the global temperature will rise by 1.5 °C by 2030-2052 (IPCC, 2022). At the 75th United Nations General Assembly, China pledged to adopt stronger policies and measures to strive for carbon neutrality by 2060. Based on China's resource endowment, the power industry is the largest source of CO_2 emissions. It is expected that coal-fired power generation will still play an irreplaceable role in China's energy structure in the future.

Carbon emissions capture, utilization, and sequestration (CCUS) technologies can capture large amounts of CO_2, which is either used or stored geologically (Chu, 2009). CO_2 to hydrogen reaction technology converts CO_2 in industrial flue gas into chemicals such as methanol (Meunier et al., 2020), formic acid (Centi et al., 2013), and methane (Zabranska and Pokorna, 2018).

It achieves the massive carbon emissions reductions needed in key industries such as power, steel, cement, and chemicals at lower cost (Wei et al., 2021). About 40 CCUS demonstration projects have been put into operation or under construction in China, and it is planned to build 3 to 5 Mt CCUS full-chain demonstration projects during the "14th Five-Year Plan" period (Cai et al., 2021). With industrial-scale applications of CCUS, the increase in supply chain networks inevitably brings many major challenges (Zhang et al., 2020). It includes scale and economics of CO_2 (Hepburn et al., 2019), optimal linkage of CCUS supply chain network sources and utilization/storage (Hasan et al., 2014), and perceptions of public perceptions of CCUS technologies (Chen et al., 2015).

The Chinese State Council's "13th Five-Year Plan" Work Plan for Greenhouse Gas Emissions Control proposed to promote industrial pilot demonstrations of CCUS systems and the corresponding environmental risk assessment (SCC, 2016). The exchange of materials and natural resources creates a "media shift" from environmental concerns to worker health and safety concerns (Ashford,1997). However, most of the current research focuses on the environmental impact of CCUS supply chain network. For example, the life cycle

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environmental impact of CCUS technologies has been assessed (Cuéllar-Franca and Azapagic, 2015). Safety risks are mainly evaluated for separate modules in the CCUS system, such as the evaluation of CO_2 sequestration leakage risks (Wei et al., 2011). Few work have studied the safety risk of CCUS supply chain networks.
This study evaluates the potential safety risks of regional CCUS system based on process simulation. A supply chain process model based on Aspen Plus simulator is established. A comprehensive inherent safety index evaluation system is proposed to quantify the safety risk of regional CCUS system.
The chemical inherent safety index, process inherent safety index, and equipment inherent safety index of a single CCUS module are compared. This study aims to identify the modules with the greatest risk in the regional CCUS system from an overall perspective, to conduct targeted safety management to reduce overall impact. The research objectives are: (1) For the existing CCUS module, a module-scale process model is established based on Aspen Plus simulaiton. An entire CCUS supply chain-scale system is investigated. (2) For safety risk assessment of the CCUS system, a comprehensive inherent safety index system is proposed based on the chemicals, process parameters, process equipment, and system structure dimensions. The framework is shown in Figure 1.

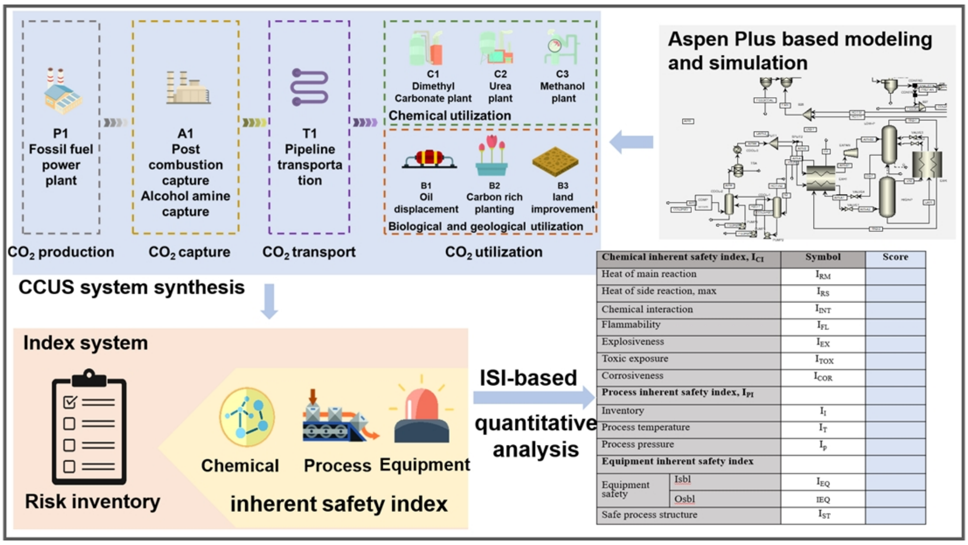

Figure 1: CCUS safety risk assessment model

2. Methods

The Chinese government clearly proposes to do a good job in the environmental risk assessment of CCUS. Due to the extension of the regional industrial chain, environmental risks are transferred to the medium of safety risks. In addition, in view of the characteristics of the CCUS industry itself, there are still difficulties such as the difficulty of quantitative evaluation, the lack of standards for critical quantities of hazardous substances, and the difficulty in obtaining basic data. Therefore, a method for quantitatively evaluating the regional CCUS industry chain is needed.

2.1 Build a comprehensive index system of inherent safety

Based on the Prototype Inherent Safety Index (PIIS) (Edwards and Lawrence,1993), this work constructs a comprehensive index system of inherent safety. Compared with PIIS, equipment safety indicators are added in addition to the chemical and process evaluation systems. Based on the process simulation, the parameters are assigned to different intervals. The overall inherent safety index is calculated as $\mathrm{ISI} = \mathrm{I_{CI}} + \mathrm{I_{PI}} + \mathrm{I_{EI}}$. The larger the ISI value, the more dangerous the module is. The specific evaluation indices are shown in Table 1.

2.2 Build a regional CCUS system model with Aspen Plus

The physical property data of each module of the CCUS system are selected using Aspen Plus. For different process systems, the unit operation modules of actual equipment are simulated. The materials, reaction heat, gas-phase composition, flow rate, temperature, pressure, and other information of different module processes are obtained to support quantitative data for subsequent safety evaluation. The fluid packages are shown in Table 2.

Table 1: Inherent Safety Index

ISI	Index	Interval		Score
Chemical inherent safety index, I_{CI}	Heat of main reaction , I_{RM} / Heat of side reaction, I_{RS}	Thermally neutral ≤200 J/g		0
		Mildly exothermic <600 J/g		1
		Moderately exothermic <1,200 J/g		2
		Strongly exothermic <3,000 J/g		3
		Extremely exothermic ≥3,000 J/g		4
	Chemical interaction, I_{INT}	Heat formation		1-3
		Fire		4
		Formation of harmless, nonflammable gas		1
		Formation of toxic gas		2-3
		Formation of flammable gas		2-3
		Explosion		4
		Rapid polymerization		2-3
		Soluble toxic chemicals		1
	Flammability, I_{FL}	Nonflammable		0
		Combustible (flash point >55℃)		1
		Flammable (flash point ≤55°C)		2
		Easily flammable (flash point <21°C)		3
		Very flammable (flash point <0°C & boiling point ≤35°C)		4
	Explosiveness (UEL-LEL) vol% , I_{EX}	Non-explosive		0
		0-20		1
		20-45		2
		45-70		3
		70-100		4
	Toxic limit (ppm), I_{TOX}	TLV > 10,000		0
		TLV≤10,000		1
		TLV≤1,000		2
		TLV≤100		3
		TLV≤10		4
		TLV≤1		5
		TLV≤0.1		6
	Construction material required, I_{COR}	Carbon steel		0
		Stainless steel		1
		Better material needed		2
		$I_{CI} = I_{RM,max} + I_{RS,max} + I_{INT} + (I_{FL} + I_{EX} + I_{TOX})_{max} + I_{COR,max}$		
Process inherent safety index, I_{PI}	Inventory, I_I	ISBL	OSBL	
		0-1t	0-10t	0
		1-10t	10-100t	1
		10-50t	100-500t	2
		50-200t	500-2000t	3
		200-500t	200-5,000t	4
		500-1,000t	5,000-10,000t	5
	Process temperature, I_T	< 0 °C		1
		0–70 °C		0
		70–150 °C		1
		150–300 °C		2
		300–600 °C		3
		>600 °C		4
	Process pressure, I_P	0.5–5 bar		0
		0–0.5 or 5–25 bar		1
		25–50 bar		2
		50–200 bar		3
		200–1,000 bar		4
	Safety level of process structure, I_{ST}	Recommended (safety etc. standard)		0
		Sound engineering practice		1
		No data or neutral		2
		Probably unsafe		3
		Minor accidents		4
		Major accidents		5
		$I_{PI} = I_I + I_T + I_P + I_{TST}$		

Table 1: Inherent Safety Index (continued)

ISI	Index		Interval	Score
Equipment inherent safety index, I_{EI}	Equipment items, I_{EQ}	inside battery limits area (Isbl)	Equipment handling nonflammable, nontoxic materials	0
			Heat exchangers, pumps, towers, drums	1
			Air coolers, reactors, high hazard pumps	2
			Compressors, high hazard reactors	3
			Furnaces, fired heaters	4
		outside battery limits area (Osbl)	Equipment handling nonflammable, nontoxic materials	0
			Atmospheric storage tanks, pumps	1
			Cooling towers, compressors, blowdown systems, pressurised or refrigerated storage tanks	2
			Flares, boilers, furnaces	3
			$I_{EI} = I_{EQ}$	

Table 2: Fluid packages

Name	P1	A1	C1	C2	C3
Fluid packages	PR-BM	PSRK	NCRL	NCRL	NCRL

3. Case study

This work takes a city in Shandong Province as an example. As shown in Figure 2, based on the actual situation, the city has a small coal gasification power plant P1, and adopts the post-combustion capture alcohol amine method A1 and pipeline transportation T1. In terms of CO_2 chemical utilization, the city has three chemical plants: dimethyl phosphate plant C1, urea plant C2, and methanol plant C3. In terms of CO_2 biological and geological utilization, it has three modules: CO_2 flooding B1, carbon-rich planting B2 and saline-alkali land improvement B3. It is assumed that they can form a systematic CCUS industry chain in the future, assess their existing environmental risks, and make risk maps for more targeted safety management.

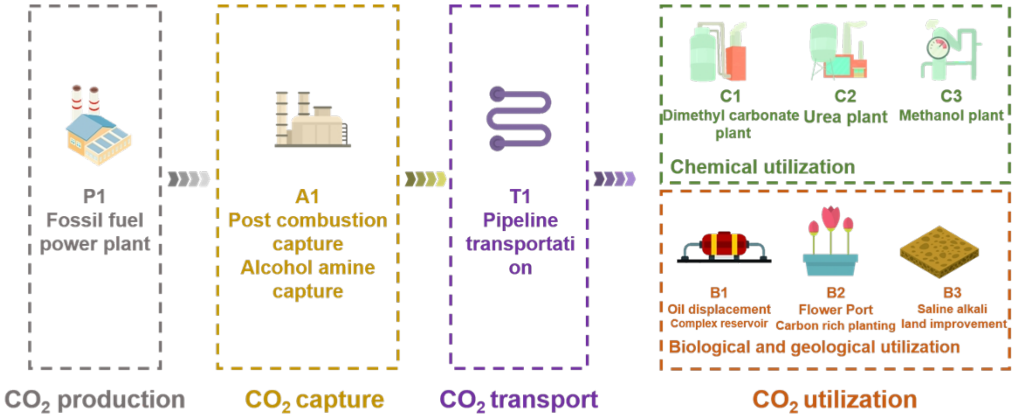

Figure 2: Modules of regional CCUS system in Dongying

The CCUS source-sink matching system is related to factors such as economic cost, geology, engineering practice, laws, and regulations. To simplify the model and ensure its rationality of the model, the following assumptions are presented:

a) The CO_2 emitted by the power plant emission source is transported to the capture point for centralized capture through pipelines;

b) Different CO_2 utilization measures require different concentrations, pressures, and temperatures, etc. It is assumed that the valve chamber at the end of the pipeline has been processed to meet the utilization requirements.

Each module of CCUS is modelled by Aspen Plus. The safety evaluation of each module is carried out using the comprehensive evaluation method of inherent safety. Aspen Plus based modules are shown in Figure 3.

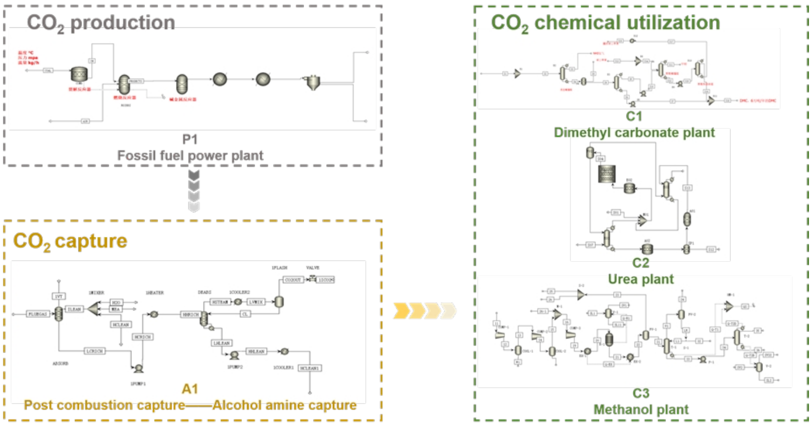

Figure 3: Regional CCUS System based on Aspen Plus

4. Results and discussions

Based on the ISI safety risk assessment, chemistry, process, equipment inherent safety index, and ISI inherent safety index of the CO_2 emission source, capture, transportation, and utilization modules are shown in Figure 4. Figure 4 shows the inherent safety index of each link of the regional CCUS system. The I_{CI} of CO_2 production module, capture module and chemical utilization module is significantly higher than I_{PI} and I_{EI}. The above modules involve chemical reactions such as coal combustion, complex amine absorption of CO_2, and synthesis of chemical products. Various chemicals and chemical processes increase the toxicity, flammability and explosiveness of modules. On the other hand, the I_{PI} of the CO_2 transport module and the geological utilization module is higher than that of the I_{CI} and I_{EI}. Specific conditions of temperature and pressure characterize the above modules. Pressure equipment and facilities such as pressure vessels and pressure pipelines are prone to physical explosions. The total safety index of the regional CCUS system modules is compared. The total safety index of the CO_2 production module is 1.52 times that of the capture module, 1.33 times that of the chemical utilization module, 2.67 times that of the transport module, and 2.67 times that of the biological/geological utilization module. This is because the emission module involves coal combustion, the process conditions are high, and there are flammable, explosive and toxic gases such as H_2, CO, and CH_4. in the process, and there are dangerous factors such as valve, flange, joint leakage in the equipment. It involves (1) flammability and explosiveness, (2) toxicity, and (3) corrosiveness. It should focus on strengthening safety management. The second is the CO_2 chemical utilization module, the capture module and the CO_2 transport module, and the biological/geological utilization module has the lowest risk. The reason is that the CO_2 biological/geological utilization module does not involve chemical reactions, and can be operated at normal temperature and pressure, so the three inherent safety indices are not high, and it is the safest utilization method.

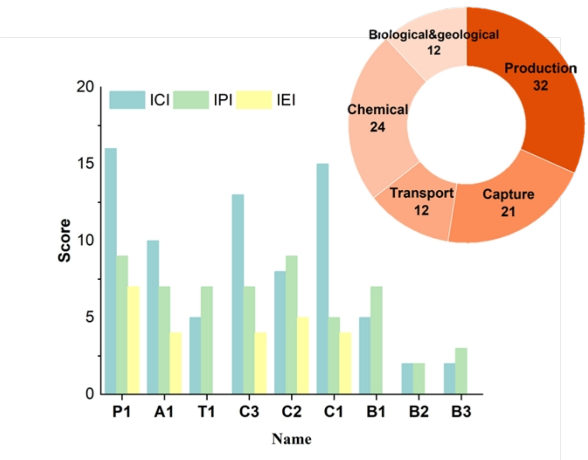

Figure 4: Risk assessment for CCUS system

5. Conclusions

A comprehensive inherent safety index evaluation method for regional CCUS systems based on Aspen Plus process simulation is proposed in this work. The risks caused by the growth of the CCUS industry chain can be investigated systematically. A CCUS system in Dongying is used as an example to illustrate the proposed method. The risk potential of each module in the regional CCUS system is classified and evaluated. The risk results are more convenient for process safety management. The total safety index of the CO_2 production module is 1.52 times that of the capture module, 1.33 times that of the chemical utilization module, 2.67 times that of the transport module, and 2.67 times that of the biological/geological utilization module. Future work can study the spatiotemporal distribution of regional CCUS systems. The deployment distribution of regional CCUS systems will be of great benefit.

Acknowledgements

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