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Method Development for the Quantitative Analysis of Hydrocarbon Impurities in Amine-Based Desulfurization Solvents

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Abstract

The antifoaming performance of natural gas desulfurization solvents is critical for maintaining product gas quality and ensuring the safe operation of processing units. Hydrocarbon impurities can enter amine solutions through feed-gas entrainment, wellhead flowback carryover, and leakage of equipment lubricants. These contaminants may gradually accumulate in the solvent system and become a significant contributor to foaming. To address the industrial demand for rapid quantitative determination of hydrocarbon contaminants in desulfurization solvents, this study investigates in-service UDS-series solvents and representative samples collected from a natural gas purification plant in western Sichuan. NMR spectroscopy and GC-MS analyses reveal that the impurities are predominantly n-alkanes in the C_{13}-C_{18} range, based on which a corresponding reference standard oil was prepared. COSMO-RS calculations combined with molecular interaction analysis identify n-hexane as the optimal extraction solvent. The ultraviolet spectrophotometric method commonly used to determine hydrocarbons in environmental water samples shows limited sensitivity to long-chain n-alkanes and requires strong acid pretreatment that disrupts the amine solvent matrix, rendering it unsuitable for UDS solvents. In contrast, the n-hexane extraction-GC-FID method showed good linearity, precision, and accuracy, meeting engineering analytical requirements for monitoring hydrocarbon contamination in MDEA-based UDS desulfurization solvents.

Keywords: desulfurization solvent; hydrocarbon impurities; analytical determination

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1. Introduction

With the global transition toward a low-carbon energy structure, natural gas, which has the lowest carbon emission intensity per unit calorific value among fossil fuels, has steadily increased its share in primary energy consumption [1,2]. However, raw natural gas commonly contains H_2S, CO_2, and organic sulfur compounds. To mitigate environmental pollution and equipment corrosion, desulfurization and purification are therefore indispensable steps in natural gas processing. Among the available purification technologies,

absorption using regenerable alkanolamine solvents remains the dominant approach owing to its technological maturity, operational flexibility, and proven reliability [3]. In industrial practice, the engineering performance of desulfurization solvents is determined not only by their sulfur removal efficiency and regeneration energy demand but also, critically, by their antifoaming performance, which directly affects the safe and stable operation of processing units. Once foaming occurs in an amine solvent system, multiple operational risks may arise. Foam entrainment can lead to severe liquid carryover and substantial solvent losses, whereas abnormal conditions such as flooding and column surging may cause pressure fluctuations and a sharp decline in processing capacity. In severe cases, foaming may even compromise product gas specifications, accelerate equipment corrosion, and result in unplanned shutdowns, thereby causing significant safety and economic losses [4,5]. Consequently, effective control of foaming in amine solvent systems remains a critical challenge for natural gas purification facilities.

Industrial practice indicates that foaming in amine solvent systems arises from multiple sources and often exhibits cumulative effects, among which the intrusion and accumulation of hydrocarbon impurities constitute a major contributing factor [6–9]. During various stages of gas field production and processing, hydrocarbon contaminants may continuously enter the desulfurization solvent system through several pathways, including condensates or heavy hydrocarbons entrained in the feed gas, oily components carried by wellhead liquid production and flowback fluids, and trace leakage of compressor lubricating oils. In real lean desulfurization solvent samples, the hydrocarbon level is not fixed and depends strongly on operating conditions. Under normal operation, upstream separation and flashing remove part of the free hydrocarbons, so a visible hydrocarbon phase is generally not observed in routine lean-solvent samples. Under abnormal conditions, such as flowback-fluid carryover into the desulfurization unit, the hydrocarbon content in the solvent can increase markedly. These heavy hydrocarbons, predominantly composed of long-chain alkanes, can significantly alter the interfacial properties of the amine solution, reduce its resistance to foaming, and under gas–liquid countercurrent contact conditions, initiate or intensify foam formation and stabilization. At present, foaming control in oil-contaminated amine systems mainly relies on passive mitigation strategies, such as the addition of antifoaming agents, physical oil removal, or online solvent drainage [10–13]. However, these approaches essentially represent post-remediation strategies. Passive control not only introduces potential complications, including additive interference, increased solvent losses, and compatibility issues within the solvent system, but also fails to provide effective dynamic monitoring or early warning of hydrocarbon accumulation during operation.

Transitioning from passive defoaming to proactive prevention and control requires the development of rapid quantitative analytical methods capable of supporting real-time evaluation and process management of hydrocarbon contaminants in desulfurization solvents. However, currently available standard methods for petroleum hydrocarbons are mainly designed for environmental water matrices, and no publicly available standardized method has been established specifically for quantifying hydrocarbon impurities in amine-based desulfurization solvent matrices. Desulfurization amine solutions typically contain various organic amines and additives and therefore exhibit strong polarity and alkalinity. This complex organic matrix can significantly interfere with conventional analytical techniques, leading to substantial limitations when existing environmental analytical methods are directly applied to natural gas desulfurization systems, including weak analytical responses and poor methodological adaptability.

To address the aforementioned industrial challenge, this study investigates in-service UDS-series composite desulfurization solvents and representative process samples collected from a natural gas purification plant in western Sichuan, China, with the aim of

developing a rapid quantitative analytical method for hydrocarbon impurities in MDEA-based UDS desulfurization solvents. First, field samples were collected and enriched, and the composition and molecular characteristics of foaming-inducing hydrocarbons present in the industrial system were elucidated through combined NMR and GC-MS analyses. Based on these results, a corresponding reference standard oil was prepared. Subsequently, using a representative heavy hydrocarbon component (n-hexadecane) and the amine solvent matrix (MDEA) as model compounds, molecular-level theoretical calculations were introduced to systematically evaluate the extraction thermodynamics and selectivity of several commonly used solvents, including n-hexane, cyclohexane, petroleum ether, and dichloromethane. This analysis enabled the identification of the optimal extractant from a mechanistic perspective. Finally, with reference to the Chinese national standards HJ 970–2018 and HJ 894–2017 [14,15], a quantitative analytical method based on n-hexane extraction coupled with gas chromatography was established and systematically validated. This work therefore adapts water-matrix petroleum hydrocarbon analysis to a complex MDEA-based UDS solvent matrix and validates the procedure using field-derived hydrocarbon compositions. The proposed method provides a practical analytical approach for quantifying hydrocarbon contaminants in MDEA-based UDS desulfurization solvents and supports rapid solvent-contamination assessment in natural gas purification units.

2. Experimental Section

2.1. Reagents and Materials

Fresh UDS desulfurization solvent was provided by Shandong Jinlu Environmental Protection Technology Co., Ltd. (Jining, China). UDS is a proprietary MDEA-based blended solvent developed for the removal of acid gases and organosulfur compounds from natural gas. The formulation contains water, N-methyldiethanolamine (MDEA), and functional components such as a five-membered sulfur-containing heterocyclic compound and a cyclic amine. The detailed formulation and component ratio of the UDS solvent were not disclosed because of industrial confidentiality. In the undiluted UDS formulation, MDEA accounts for more than 70% of the solvent components and serves as the dominant amine matrix. Therefore, MDEA was selected as the representative amine matrix in the theoretical screening of extractants. In this study, the fresh solvent was diluted with deionized water to an industrial working concentration of 45 wt% and used as the representative UDS working solution for method development and validation. For natural-gas amine absorption units, the absorber temperature is commonly around 30–50 °C, and the operating pressure is typically in the MPa range. A field DCS record during sampling showed an absorber pressure of approximately 4.6 MPa.

n-Hexane, n-tetradecane, n-pentadecane, n-hexadecane, n-heptadecane, n-octadecane, and anhydrous sodium sulfate were all of analytical grade and purchased from Shanghai Macklin Biochemical Co., Ltd. (Shanghai, China). n-Hexane was used as the extraction solvent, and anhydrous sodium sulfate was used to dry the organic extracts. The five linear n-alkanes from n-C14 to n-C18 were used to prepare the reference standard oil according to the hydrocarbon composition identified in field samples. Gasfield water samples were supplied by a natural gas purification plant in western Sichuan, China. Nitrogen with a purity of 99.999% was supplied by Shanghai Wetry Standard Gas Analysis Technology Co., Ltd. (Shanghai, China).

2.2. Characterization and Analysis

Hydrocarbon impurities present in gasfield water were identified using ^{1}H nuclear magnetic resonance (^{1}H NMR) spectroscopy. The measurements were conducted at room temperature on a Bruker Ascend 600 NMR spectrometer (Bruker BioSpin GmbH, Rhe-

instetten, Germany). Each spectrum was obtained by averaging 512 scans. Deuterated chloroform ($CDCl_3$) was used as the solvent, and the chemical shift was referenced to 7.26 ppm.

The composition of hydrocarbon impurities was further analyzed using GC-MS. The analysis was performed at room temperature on an Agilent 7890A GC-5975 MS system (Agilent Technologies, Inc., Santa Clara, CA, USA). The chemical components were identified by comparing the total ion chromatogram (TIC) with the NIST mass spectral database, while the relative composition was evaluated based on retention times and peak areas.

The quantitative determination of hydrocarbons in the extracts and concentrated extracts was carried out using an Agilent 7890B gas chromatograph (Agilent Technologies, Inc., Santa Clara, CA, USA). The instrument was equipped with an HP-5 capillary column (30 m × 0.25 mm × 0.25 μm), a flame ionization detector (FID), and an electronic pneumatic control (EPC) injection system. The GC operating conditions were as follows: injector temperature, 280 °C; carrier gas flow rate, 2.0 mL min^{-1}; oven temperature program, initially 60 °C (2 min), increased to 280 °C at 15 °C min^{-1}, and held for 15 min. The FID temperature was 300 °C, with hydrogen, air, and make-up gas flow rates of 40.0, 350.0, and 30.0 mL min^{-1}, respectively.

Petroleum hydrocarbons in the solvent were also analyzed using UV-vis spectrophotometry. Measurements were performed at room temperature on a Lambda 750S UV-vis-NIR spectrophotometer (PerkinElmer, Inc., Shelton, CT, USA) using a 2 cm quartz cuvette. The scanning wavelength range was 200–300 nm, and the absorbance mode was employed. n-Hexane was used as the blank reference. The petroleum hydrocarbon content was determined from the established calibration curve based on the measured absorbance according to the Beer-Lambert law.

2.3. Theoretical Calculations

The conductor-like screening model for real solvents (COSMO-RS) was employed to evaluate the thermodynamic interactions between solutes and solvents [16,17]. The infinite-dilution activity coefficients (γ_i^∞) of solutes in different solvents were calculated using the Activity Coefficient Calculation module in COSMOthermX (version 19.0.4). All COSMO files were generated from quantum chemical calculations performed with Gaussian 09 at the BP86/TZVP level of theory. The solvent capacity (C^∞) and selectivity (S^∞) were subsequently determined according to Equations (1) and (2), respectively [18].

$$C_i^\infty = \frac{1}{\gamma_i^\infty} \tag{1}$$

$$S^\infty = \frac{C_1^\infty}{C_2^\infty} \tag{2}$$

where γ_i^∞ represents the activity coefficient of the solute in the solvent at infinite dilution. The performance index (PI^∞), defined by Equation (3), is used to describe the overall extraction efficiency of the solvent under infinite-dilution conditions.

$$PI^\infty = C_1^\infty \times S^\infty \tag{3}$$

To investigate the influence of extractant molecular structure on separation performance and to elucidate the interaction mechanisms between solvent and solute molecules, quantum chemical calculations were performed using Gaussian 09 and GaussView 6.0. The geometries of the solute and solvent molecules were optimized, followed by vibrational frequency analyses, at the B3LYP/6-31G* level of theory. Based on the optimized structures, electrostatic potential (ESP) analyses on the molecular surfaces were conducted using the

Multiwfn 3.8 program in combination with Visual Molecular Dynamics (VMD) [19,20]. The molecular polarity index (*MPI*) was calculated according to Equation (4) [21,22]. The MPI parameter was employed to quantify the local polarity arising from the nonuniform distribution of ESP and to characterize the polarity of nonpolar molecules.

$$MPI = \left(\frac{1}{A}\right)\iint_{S}^{0} /V(\mathrm{r})/\mathrm{d}S \tag{4}$$

where A denotes the molecular surface area (Å^2), and V(r) represents the electrostatic potential at a given point, expressed in kcal mol^{-1}.

The Molclus program was employed to identify the most stable configurations for each solvent-solute system. A total of 50 initial dimer conformations were randomly generated for each binary molecular pair to sample all possible relative intermolecular orientations [23]. These dimer structures were subsequently optimized using Gaussian 09, followed by vibrational frequency analyses at the B3LYP/6-31G* level of theory. The initial geometries of the isolated monomers were also optimized, and their single-point energies were calculated at the same theoretical level. The interaction energies (E_{int}) between the molecules in different dimers were then calculated according to Equation (5), and the results were corrected for basis set superposition error (BSSE).

$$E_{int} = E_{AB} - E_A - E_B + E_{BSSE} \tag{5}$$

where E_{AB} represents the total energy of the binary molecular complex, while E_A and E_B correspond to the energies of the isolated solvent and solute molecules, respectively. E_{BSSE} denotes the energy correction for basis set superposition error, expressed in kJ mol^{-1}.

The independent gradient model based on Hirshfeld partition (IGMH) was further employed to visualize intermolecular interactions. The regions of intermolecular interactions with different strengths were characterized using the δg function [24]. This analysis enables the identification of the location, type, and relative strength of interactions between the solute and solvent molecules.

3. Results and Discussion

3.1. Analysis of Hydrocarbon Impurities in Gasfield Water and Preparation of Reference Standard Oil

Gasfield water samples were collected from the outlet of the SN-102 stripping tower at processing stations No. 4, 5, and 6 of the Pengzhou gas field (Figure 1a). The gasfield water contained liquid-phase impurities introduced by wellbore flowback fluids as well as liquid hydrocarbon components entrained in the raw natural gas. A distinct oil-water phase separation was observed in the sample from station No. 5. To accurately determine the composition and content of heavy hydrocarbons in the flowback mixture, the oil phase in the samples was enriched and concentrated prior to analysis. Considering the strong extraction selectivity of n-hexane toward high-carbon-number alkanes, liquid–liquid extraction was performed using three portions of 50.0 g n-hexane to extract 100.0 g of the gasfield water sample. Each extraction was conducted in a separatory funnel with vigorous shaking followed by phase separation. The three organic phases were collected and combined, and the solvent was removed by rotary evaporation at 55 °C to obtain a concentrated extract for subsequent compositional analysis (Figure 1b).

The major components in the concentrated extract were qualitatively identified using ^{1}H NMR spectroscopy, as shown in Figure 1c. $CDCl_3$ containing an internal reference was used as the solvent, with the chemical shift referenced to 7.26 ppm. The signals at approximately 0.9 ppm and 1.2 ppm correspond to the proton resonances of methyl

($-CH_3$) and methylene ($-CH_2$) groups in hydrocarbon compounds, respectively, while the signal near 5.0 ppm is attributed to residual water or hydroxyl protons (-OH) from trace alcohols. The ^{1}H NMR results indicate that the oil-like impurities introduced into the gasfield water and raw natural gas by wellbore flowback fluids are predominantly hydrocarbon compounds. To further determine the composition and distribution of these hydrocarbons, the concentrated extract was analyzed using GC-MS, and the results are presented in Figure 1d. Individual components were identified by comparison with the NIST mass spectral database, and their relative compositions were determined by peak integration using the FID detector. The main hydrocarbon impurities are summarized in Table 1, which shows that the contaminants are primarily n-alkanes with carbon numbers ranging from C_{13} to C_{18}. These hydrocarbons are introduced into the desulfurization system through gasfield water or raw natural gas, leading to contamination of the UDS solvent. The presence of these impurities alters the surface tension and viscosity of the lean solvent, thereby deteriorating the desulfurization efficiency and antifoaming performance of the amine system.

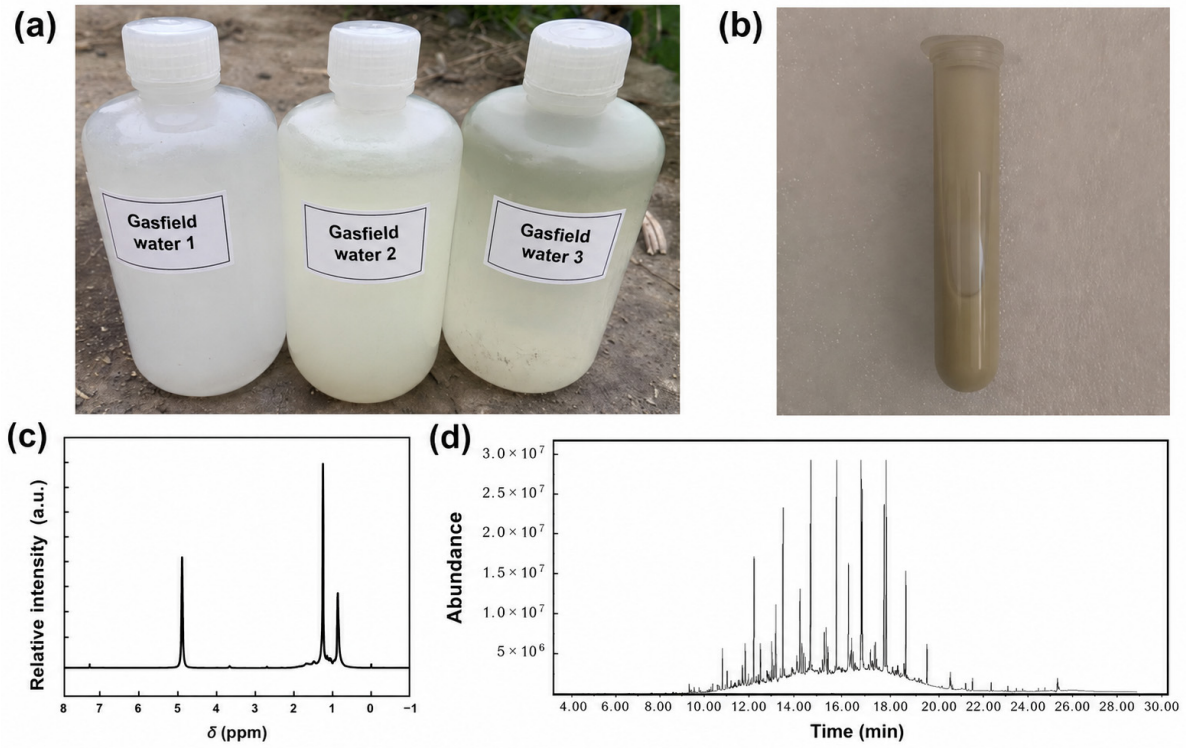

Figure 1. Field sampling of gasfield water from the Pengzhou gas field and analysis of hydrocarbon impurities: (**a**) on-site sampling photograph; (**b**) concentrated extract of oil-phase impurities from gasfield water; (**c**) ^{1}H NMR spectrum of the concentrated extract; (**d**) GC-MS chromatogram of the concentrated extract.

Table 1. Composition of major hydrocarbon impurities in gasfield water.

No.	Compound	Mass Fraction (%)	CAS No.
1	Decane	0.05	124-18-5
2	Undecane	0.306	1120-21-4
3	4-Methyldecane	0.099	2847-72-5
4	Dodecane	1.467	112-40-3
5	2,6-Dimethylundecane	0.727	17301-23-4
6	5-Butyl-4-nonene	1.129	7367-38-6

Table 1. *Cont.*

No.	Compound	Mass Fraction (%)	CAS No.
7	7-Methyltridecane	1.665	26730-14-3
8	Tridecane	4.53	629-50-5
9	2-Methyltridecane	3.538	1560-96-9
10	2,6,10-Trimethyldodecane	2.036	3891-98-3
11	Tetradecane	6.521	629-59-4
12	2,7,10-Trimethyldodecane	5.336	74645-98-0
13	n-Pentadecane	8.469	629-62-9
14	2-Methylpentadecane	6.756	1560-93-6
15	n-Hexadecane	9.063	544-76-3
16	2,6,10-Trimethyltetradecane	8.49	14905-56-7
17	n-Heptadecane	8.656	629-78-7
18	Pristane	5.806	1921-70-6
19	n-Octadecane	6.519	593-45-3
20	Phytane	8.621	638-36-8
21	n-Heneicosane	3.232	629-94-7
22	n-Eicosane	1.208	112-95-8
23	n-Heptacosane	0.36	593-49-7

To establish a quantitative analytical method for hydrocarbon impurities in UDS solvents under the actual production conditions of the Pengzhou gas field, representative components were selected for the preparation of the standard oil. As shown in Table 1, the impurity composition is relatively complex, including various structural types such as n-alkanes and branched alkanes, among which n-alkanes in the C_{13}–C_{18} range exhibit the highest abundance and diversity. Considering the component content, structural representativeness, and commercial availability of reagents, five high-abundance n-alkanes (n-tetradecane, n-pentadecane, n-hexadecane, n-heptadecane, and n-octadecane) were ultimately selected as the standard oil components (Table 2). These hydrocarbons possess stable structures and are readily amenable to analysis, while also being consistent with the dominant impurity types observed in field samples, thereby improving the quantitative accuracy and practical applicability of the proposed method.

Table 2. Composition of the standard oil.

Compound	CAS No.	Content in Gasfield Water (%)	Content in Standard Oil (%)
n-Tetradecane	629-59-4	6.521	16.67
n-Pentadecane	629-62-9	8.469	21.79
n-Hexadecane	544-76-3	9.063	23.08
n-Heptadecane	629-78-7	8.656	21.79
n-Octadecane	593-45-3	6.519	16.67

3.2. Theoretical Screening and Selection of Extractants

To establish a rapid quantitative analytical method for hydrocarbon impurities in MDEA-based UDS desulfurization solvents, the national environmental protection standards HJ 970–2018 and HJ 894–2017 were referenced. Both standards are based on the principle of organic solvent extraction followed by subsequent analytical characterization. However, unlike these standard methods that are primarily designed for environmental water samples such as surface water and seawater, the desulfurization amine solutions employed in natural gas purification are composite organic amine aqueous systems. These systems contain multiple functional organic components and exhibit strong alkalinity, high organic content, and relatively high viscosity, which impose more stringent requirements

on the selection of extraction solvents. Therefore, it is necessary to screen efficient extractants capable of selectively extracting high-carbon-number hydrocarbon impurities from such complex aqueous amine systems to ensure the accuracy and stability of subsequent quantitative analysis.

According to the recommended procedures in standard methods and relevant literature [16–18], commonly used extractants include n-hexane, cyclohexane, petroleum ether (mainly composed of n-pentane), and dichloromethane. To evaluate the suitability of these extractants in the target system, n-hexadecane was selected as a representative model compound for hydrocarbon impurities, while N-methyldiethanolamine (MDEA) was used as the representative amine solvent matrix. COSMO-RS and quantum-chemical interaction analysis have been used for solvent screening, extraction-separation evaluation, and amine-based gas absorption systems. Here, these methods were used as supporting tools to evaluate extractant suitability for the field-derived long-chain hydrocarbon profile and the MDEA-based UDS solvent matrix, rather than to propose a new theoretical model. The extraction performance of different solvents was compared through theoretical calculations to select a suitable organic solvent for extracting hydrocarbon impurities from the MDEA-based UDS solvent matrix.

To preliminarily evaluate the feasibility of different extractants in the target solvent system, the COSMO-RS model was employed to predict the solubility and selectivity of n-hexadecane and MDEA in n-hexane, cyclohexane, n-pentane, and dichloromethane (Table 3). The solvent capacity (C^{∞}) reflects the solubility of the solute in the extractant, where a higher C^{∞} indicates that a smaller amount of solvent is required to achieve effective extraction. In contrast, the selectivity (S^{∞}) represents the separation capability of the solvent toward the target system; a higher S^{∞} suggests easier separation and a higher purity of the extracted component in the organic phase. An ideal solvent should therefore exhibit both high C^{∞} and S^{∞} values. In this study, the performance index (PI^{∞}) was adopted as a comprehensive indicator to evaluate the extraction efficiency, where a larger PI^{∞} value corresponds to a more effective extractant. The predicted extraction performance of the four solvents toward n-hexadecane follows the order: cyclohexane > n-pentane > n-hexane > dichloromethane. Except for dichloromethane, the other three solvents exhibit relatively favorable extraction capabilities. In practical industrial applications, however, solvent selection must consider not only extraction performance but also safety and environmental compatibility. Although cyclohexane and n-pentane show promising extraction performance, both present potential operational risks. Cyclohexane is a volatile organic compound with certain toxicity and may pose health hazards under long-term exposure or poorly ventilated conditions, potentially causing neurological damage [25]. In addition, n-pentane possesses an extremely low boiling point and high vapor pressure, leading to rapid volatilization at ambient conditions. This may result in significant solvent loss during extraction, making quantitative analysis difficult, and may also increase the risk of fire and explosion due to the formation of flammable vapors. Considering these factors comprehensively, n-hexane was selected as the preferred solvent for extracting hydrocarbon impurities from the MDEA-based UDS solvent matrix because it combines satisfactory extraction performance with practical operational safety.

Beyond the prediction of thermodynamic solubility, ESP and MPI analyses were used to compare the polarity matching between the candidate extractants, n-hexadecane, and MDEA. The optimized molecular structures, ESP distributions, and *MPI* values of the solvents and solutes are presented in Figure 2. In the ESP maps, red and blue regions correspond to positive and negative electrostatic potentials, respectively, while the local maxima and minima are indicated by yellow and cyan points. As shown in Figure 2, n-hexane, cyclohexane, n-pentane, and n-hexadecane exhibit relatively low polarity with a

nearly uniform distribution of positive and negative electrostatic potentials. In contrast, dichloromethane displays a pronounced dipole character, where the regions surrounding the Cl atoms are dominated by negative electrostatic potential, while the central region exhibits positive potential. For MDEA, distinct polar regions are observed on the molecular surface: the vicinity of the N atom presents a strong negative electrostatic potential, whereas the -OH groups exhibit positive potential, indicating the relatively strong polarity of the molecule. The *MPI* value was employed as a quantitative descriptor of the overall molecular polarity. Solvation behavior is primarily governed by the polarity compatibility between solvent and solute molecules. Compared with MDEA, the *MPI* values of n-hexane, cyclohexane, and n-pentane are closer to those of n-hexadecane, suggesting a stronger solvation tendency for n-hexadecane in these solvents. In contrast, MDEA exhibits a higher solvation tendency in dichloromethane, consistent with its relatively higher polarity.

Table 3. COSMO-RS-predicted solvent capacity (C^{∞}), selectivity (S^{∞}), and performance index (PI^{∞}) of n-hexadecane and MDEA in four extractants at infinite dilution (273.15 K).

Solvent	C_1^{∞}	C_2^{∞}	S^{∞}	PI^{∞}
n-Hexane	1.25442	0.00022	5638.20522	7072.65366
Cyclohexane	1.39846	0.00021	6547.74883	9156.73964
n-Pentane	1.39128	0.00022	6392.97954	8894.45360
Dichloromethane	0.11899	0.03311	3.59382	0.42763

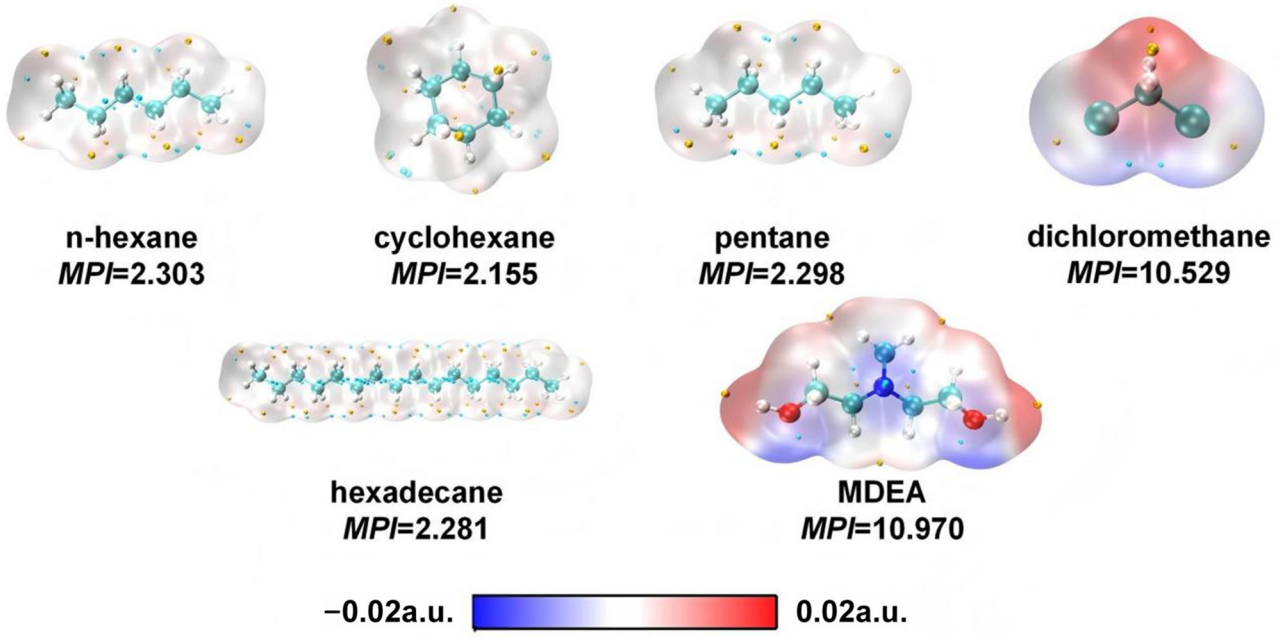

Figure 2. Optimized molecular structures, ESP distributions, and *MPI* values of the solvent and solute molecules.

The selectivity and solubility of solvents toward solutes are closely related to the intermolecular interactions within the solvent-solute system. The calculated results show that the E_{int} between n-hexane, cyclohexane, and n-pentane and n-hexadecane is significantly larger than that between these solvents and MDEA. This result indicates that these three solvents exhibit a stronger affinity for n-hexadecane. The difference in interaction energies provides a driving force for the selective separation of n-hexadecane from MDEA. In contrast, the E_{int} between dichloromethane and n-hexadecane is smaller than that between dichloromethane and MDEA, indicating that dichloromethane has a relatively weak affinity for n-hexadecane and is therefore not suitable as an extraction solvent in this

system. In addition, a larger difference in interaction energy $|\Delta E_{int}|$ between a solvent and the two solutes indicates higher separation selectivity toward the target component. Among the four solvent systems, n-hexane exhibits the largest $|\Delta E_{int}|$, indicating the highest separation selectivity.

To further elucidate the intermolecular interactions between solutes and solvents, the independent gradient model based on Hirshfeld partition (IGMH) method was employed to visualize the weak interactions in different solute-solvent systems. The isosurface maps generated at δg = 0.002 a.u. are shown in Figure 3. The isosurfaces between the extractants and solutes are predominantly green, indicating that van der Waals interactions dominate in these systems. A larger isosurface area and darker color correspond to stronger intermolecular interactions. The n-hexane + n-hexadecane system (Figure 3a) exhibits a continuous and extensive interaction region, which is more pronounced than the localized chain-ring contact observed in the cyclohexane + n-hexadecane system (Figure 3c). Compared with n-pentane (Figure 3e), n-hexane possesses a longer carbon chain, which facilitates the formation of more extended and continuous isosurface regions with n-hexadecane and promotes a more stable parallel stacking configuration. This structural feature enhances the intermolecular interactions between the two molecules. In addition, the attractive interactions between MDEA and the solvent molecules are mainly governed by C-H···O interactions. Except for dichloromethane, the isosurface areas between the solvents and n-hexadecane are larger than those between the solvents and MDEA, which is consistent with the interaction energy analysis and further confirms the extraction selectivity of n-hexane toward n-hexadecane.

Overall, n-hexane showed favorable thermodynamic behavior and intermolecular interactions and was selected as the extraction solvent for hydrocarbon impurities in the MDEA-based UDS solvent system.

3.3. Evaluation of the UV Spectrophotometric Method

Referring to the Chinese environmental protection standard HJ 970–2018 Water Quality Determination of Petroleum Oils by Ultraviolet Spectrophotometric Method (Trial), an attempt was made to establish an analytical method for determining the oil content in UDS lean solution. This standard is mainly applicable to the determination of petroleum substances in surface water, groundwater, and seawater, and is primarily used in environmental monitoring and pollution control. The target analytes are petroleum hydrocarbons, including mineral oils and diesel-like compounds, which mainly consist of low- to medium-polarity hydrocarbons. In this method, the sample is extracted with n-hexane under pH $\leq$ 2 conditions to transfer hydrocarbon compounds into the organic phase. The extract is then dehydrated using anhydrous sodium sulfate and purified with magnesium silicate to remove interference from polar substances. The absorbance of the final solution is measured at 225 nm. According to the Lambert Beer law, the absorbance shows a linear relationship with the concentration of hydrocarbons. A calibration curve is established, and the hydrocarbon impurity content in the sample (ρ, mg/L) is calculated using Equation (6).

$$\rho = \frac{10 \cdot (A - A_0 - a) \cdot V_1}{b \cdot V} \quad (6)$$

where A is the absorbance of the sample, A_0 is the absorbance of the blank, a and b are the intercept and slope of the calibration curve, V_1 is the volume of the extract, and V is the volume of the sample.

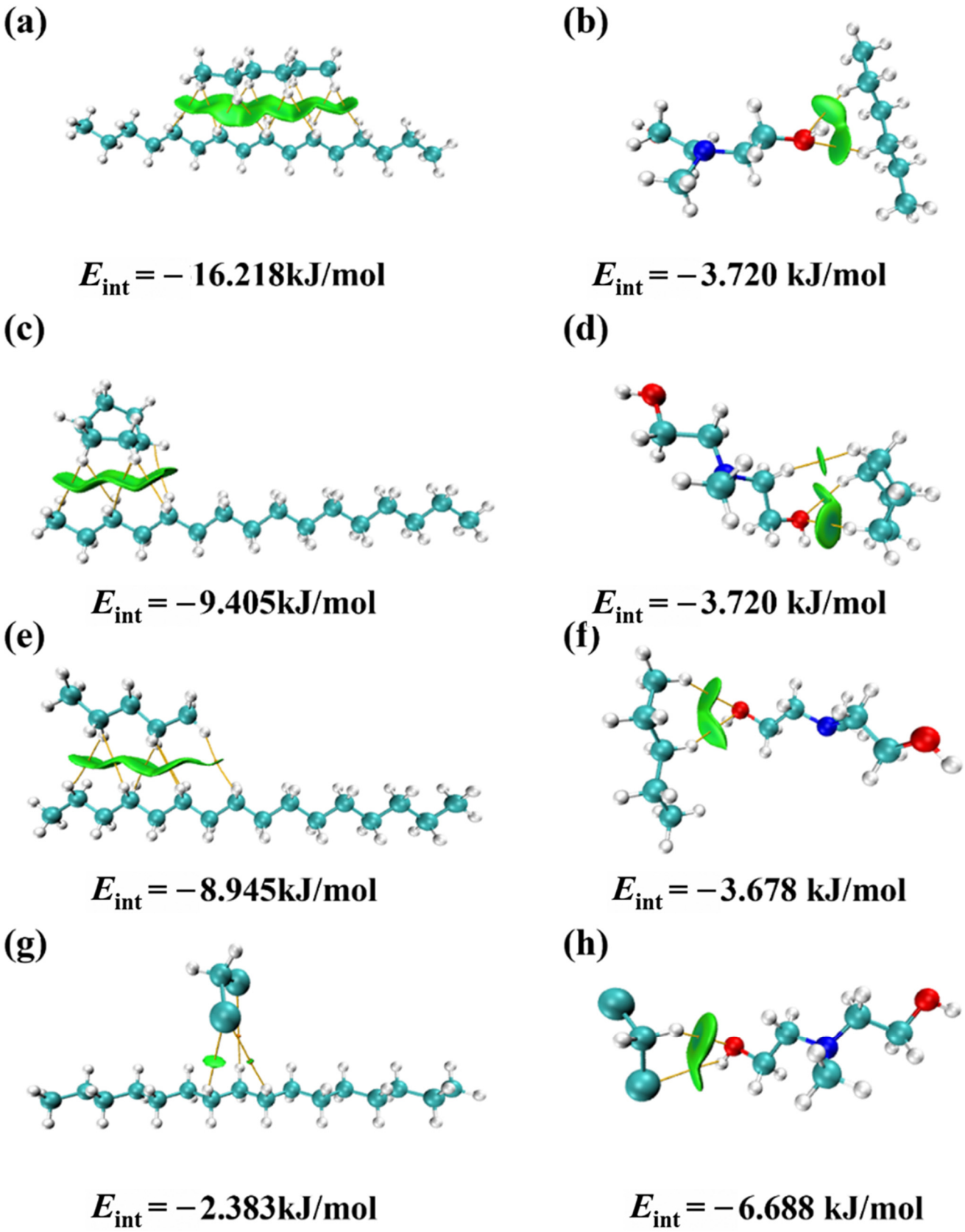

Figure 3. Interaction energy (E_{int}), IGMH isosurfaces, bond critical points (BCP), and interaction paths for different solvent-solute systems: (**a**) n-hexane + n-hexadecane; (**b**) n-hexane + MDEA, (**c**) cyclohexane + n-hexadecane; (**d**) cyclohexane + MDEA; (**e**) n-pentane + n-hexadecane; (**f**) n-pentane + MDEA; (**g**) dichloromethane + n-hexadecane and (**h**) dichloromethane + MDEA.

This method clearly requires that the transmittance of the extraction solvent n-hexane at 225 nm, using water as the blank reference, should be greater than 90%. Otherwise, a dearomatization treatment is required. In commonly used analytical grade n-hexane products from several domestic suppliers, trace amounts of aromatic compounds are generally present. These impurities exhibit strong absorption in the ultraviolet region and reduce the transmittance, resulting in values that do not meet the standard requirement and therefore cannot be directly used for extraction experiments. In order to screen suitable extraction solvents for ultraviolet detection, several chromatographic-grade or higher purity n-hexane reagents from different suppliers were selected according to the standard for testing. The relevant information is listed in Table 4.

Table 4. n-Hexane reagents used in the ultraviolet spectrophotometric method.

Code	Brand	Grade	Manufacturer	Transmittance at 225 nm (%)
A	CNW	Chromatographic grade	ANPEL Laboratory Technologies (Shanghai, China), Inc.	82.07
B	CNW	Pesticide residue grade	ANPEL Laboratory Technologies (Shanghai, China), Inc.	84.53
C	Innochem	ACS grade	Innochem (Beijing, China) Technology Co., Ltd.	81.12
D	Energy Chemical	Chromatographic grade	Anhui Senrise Technologies Co, Ltd. (Anqing, Anhui, China)	0

Figure 4a shows the transmittance results of four n-hexane samples at 225 nm. All values are lower than 90%, indicating that the method has strict requirements for reagent purity. Based on n-hexane B, which showed the transmittance closest to the standard requirement, the solvent was alternately washed three times with 5 wt% sulfuric acid and deionized water and then dehydrated using anhydrous sodium sulfate. After treatment, the transmittance at 225 nm increased to 92.35%, meeting the standard requirement and allowing the solvent to be used as the extraction agent in subsequent ultraviolet spectrophotometric determination.

In addition, the ultraviolet absorption method requires the addition of dilute sulfuric acid to the UDS lean solution sample to adjust the pH to below 2 during sample preparation. This treatment contaminates the analyzed sample and prevents the solution from being used for other solvent property tests. The treated solution also cannot be recycled after analysis. Therefore, the ultraviolet spectrophotometric method is not suitable for determining the hydrocarbon impurity content in the UDS composite desulfurization solvent from the western Sichuan gas field.

According to the requirements of the standard method, a standard oil sample was quantitatively added to a 45 wt% UDS-3 solution to prepare five series of samples with oil contents of 50 mg/kg, 100 mg/kg, 300 mg/kg, 500 mg/kg, and 700 mg/kg. The solutions were acidified with 1 wt% dilute sulfuric acid to pH $\leq$ 2 and then extracted with qualified n-hexane for liquid–liquid extraction. The absorbance of the sample solution A and the blank A_0 was recorded. The ultraviolet absorption spectra of the five extracts in the wavelength range of 200 to 300 nm are shown in Figure 4b. The results show that no obvious characteristic peak appears at the recommended wavelength of 225 nm. A weak absorption peak is observed in the range of 203 to 210 nm. However, the ultraviolet transmittance in this region is inherently low, resulting in unstable signals, and negative absorbance values are even observed for some samples. Although a partial response appears near the absorption region, the absorbance does not show a linear relationship with the hydrocarbon impurity concentration, and an effective calibration curve cannot be established. Compared with the example described in the standard method, the problem

may originate from the composition of the standard oil used in this study. The standard oil mainly consists of normal alkanes, which are low-polarity saturated hydrocarbons with weak ultraviolet absorption ability. In contrast, the standard method is more suitable for petroleum compounds such as isoalkanes, cycloalkanes, or hydrocarbons containing unsaturated bonds with relatively higher polarity. Therefore, no effective response is observed in the target wavelength region in this study.

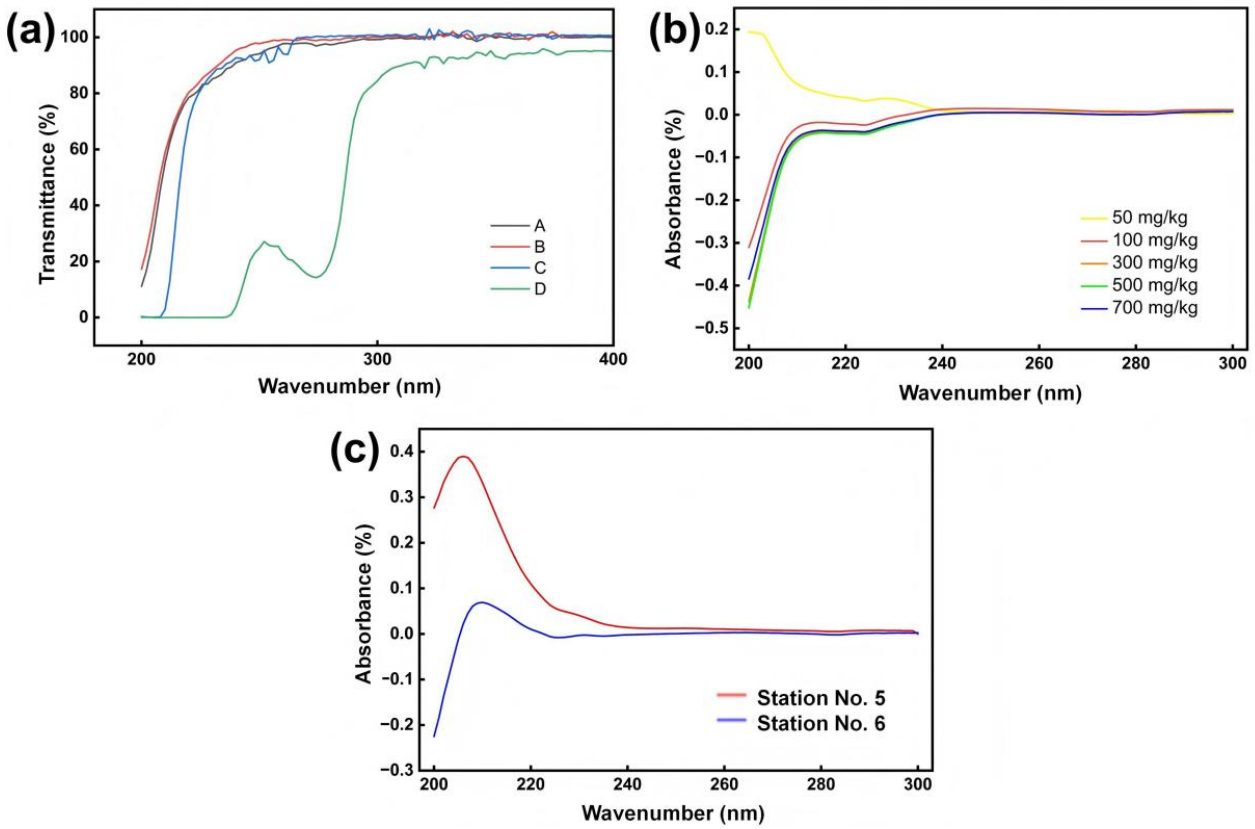

Figure 4. Ultraviolet absorption and transmittance characteristics of samples determined by the ultraviolet spectrophotometric method: (**a**) ultraviolet transmittance of n-hexane reagents; (**b**) ultraviolet absorbance spectra of n-hexane extracts of standard samples; (**c**) ultraviolet absorbance spectra of n-hexane extracts of produced water from gas treatment stations 5 and 6.

For further verification, the same ultraviolet analytical method was applied to directly extract produced water samples from gas treatment stations No. 5 and No. 6. The results are shown in Figure 4c. Weak absorption peaks appear at 206 nm and 210 nm for the two samples, respectively. This observation indicates that the hydrocarbon impurity compositions differ significantly between different stations, and their ultraviolet absorption characteristics are not consistent. As a result, the universality of this method is limited for practical applications.

3.4. Attempt to Establish an Extraction-Gas Chromatography Method

To further develop an analytical method suitable for determining hydrocarbon impurities in MDEA-based UDS desulfurization solvents, the national environmental protection standard HJ 894-2017 Water Quality Determination of Extractable Petroleum Hydrocarbons (C_{10}–C_{40}) by Gas Chromatography was referenced to establish a quantitative analysis procedure based on liquid–liquid extraction coupled with gas chromatography. This standard method is primarily applicable to the determination of extractable petroleum hydrocarbons in the C_{10}–C_{40} range in surface water, groundwater, seawater, and industrial wastewater.

The target components include medium- and low-polarity hydrocarbons such as aliphatic hydrocarbons, alicyclic hydrocarbons, and certain aromatic hydrocarbons.

In this method, petroleum substances in water samples are extracted with an organic solvent under acidic conditions with a pH $\leq$ 2. The extract is then dehydrated using anhydrous sodium sulfate, concentrated by rotary evaporation, purified using a magnesium silicate adsorbent, and finally diluted to volume with n-hexane. The prepared extract is analyzed using a gas chromatograph equipped with a flame ionization detector. Qualitative identification is carried out based on retention time, while the peak area within the defined time window is quantified using an external standard calibration curve. The hydrocarbon impurity content in the sample ρ in mg/L is calculated according to Equation (7).

$$\rho = \frac{(A_x - a) \cdot V_1}{b \cdot V \cdot f} \quad (7)$$

where A_x represents the total peak area of the sample after subtracting column bleed, a and b denote the intercept and slope of the calibration curve, respectively, V_1 is the volume of the extraction solution, V is the sample volume, and f is the dilution factor.

Referring to this standard, and considering the composition characteristics of hydrocarbon impurities in the Western Sichuan gas field as well as the specific properties of the MDEA-based UDS solvent, n-hexane was selected as the preferred extraction solvent. Standard oil masses of 0.006 g, 0.015 g, 0.030 g, 0.090 g, and 0.150 g were accurately weighed into test tubes using a high-precision balance. Each sample was then diluted to 30.00 g with n-hexane and thoroughly mixed. The resulting standard series had mass concentrations of 200 mg/kg, 500 mg/kg, 1000 mg/kg, 3000 mg/kg, and 5000 mg/kg, respectively. A calibration curve was established by plotting the mass concentration of the standard series mg/kg on the horizontal axis and the corresponding total chromatographic peak area on the vertical axis. The gas chromatogram of the standard oil is shown in Figure 5a, and the calibration curve is presented in Figure 5b. The regression coefficient of the calibration curve is greater than 0.999, which meets the requirements of the analytical method.

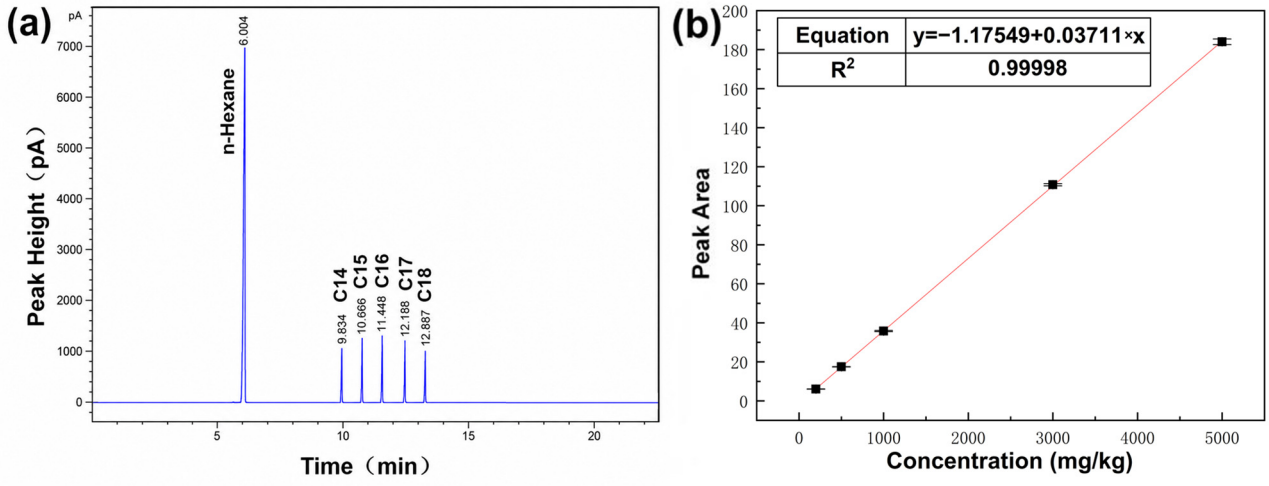

Figure 5. Gas chromatographic analysis results: (**a**) gas chromatogram of the standard oil; (**b**) calibration curve of the gas chromatography method. Error bars represent standard deviations from triplicate injections.

The concentration obtained from this calibration curve is reported as the standard-oil-equivalent total hydrocarbon concentration. Since the method targets total hydrocarbon monitoring rather than individual-component quantification, component-specific FID sensitivity coefficients were not applied. The reference standard oil was prepared from

the dominant n-C14 to n-C18 alkanes identified in field samples, making it representative of the target hydrocarbon profile. Possible response differences from branched alkanes, isoprenoid hydrocarbons, and other minor components were evaluated through the spiked-sample validation described below.

Further experiments were conducted to evaluate the precision and accuracy of the extraction-gas chromatography method. Standard oil masses of 0.025 g, 0.025 g, 0.050 g, and 0.150 g were accurately weighed and diluted with 45% desulfurization solution to a total mass of 50.00 g, yielding four samples with concentrations of 500 mg/kg, 500 mg/kg, 1000 mg/kg, and 3000 mg/kg, labeled as 1, 2, 3, and 4. Each sample was completely transferred into a 125 mL separatory funnel. Then 10 g of n-hexane, weighed to an accuracy of 0.0001 g, was used to rinse the sampling bottle and subsequently transferred into the separatory funnel. The mixture was vigorously shaken for 2 min, with the stopcock periodically opened to release pressure. After phase separation, the upper organic phase was collected as the extract, and the mass of the extract was measured and recorded. The extract was transferred into an Erlenmeyer flask containing 3 g of anhydrous sodium sulfate. The flask was sealed and shaken several times, followed by standing for phase separation. If the anhydrous sodium sulfate was completely agglomerated, additional sodium sulfate was added until no further agglomeration occurred. When the petroleum hydrocarbon content in the original sample was relatively high, the extract could be directly analyzed by gas chromatography, in which case the dilution factor f was equal to 1. If the hydrocarbon content in the original sample was low and possibly below the detection limit of gas chromatography, the extract could be concentrated to a volume not less than 1 mL using a concentration device. The recommended conditions for concentrating n-hexane were a water bath temperature of 30 °C and a vacuum of 260 hPa. The mass of the extract before and after concentration was recorded to calculate the concentration factor. A fresh UDS solution was treated following the same procedure and used as a blank control sample. Each sample was analyzed in triplicate. The mean value, relative standard deviation, and relative error were calculated for each sample. The results are presented in Table 5. The relative standard deviations of the four prepared samples ranged from 1.14% to 1.68%, and the relative errors ranged from −4.31% to 4.44%. These results indicate that the method is suitable for determining hydrocarbon impurities in MDEA-based UDS desulfurization solvents.

Table 5. Precision and accuracy results of spiked samples.

Sample		1	2	3	4
Replicate	1	481.89	482.15	1052.48	2989.81
	2	472.17	491.45	1024.24	3051.03
	3	481.35	476.34	1056.42	3059.46
Mean (mg/kg)		478.47	483.31	1044.38	3033.43
Relative standard deviation *RSD* (%)		1.14	1.58	1.68	1.25
Theoretical concentration μ (mg/kg)		500.00	500.00	1000.00	3000.00
Relative error *RE* (%)		−4.31%	−3.34%	4.44%	1.11%

Under conditions without concentration of the extract, the optimal measurement range of this method is approximately 200 mg/kg to 1000 mg/kg. When the petroleum hydrocarbon content is lower than 200 mg/kg, the gas chromatographic signal becomes weak, and the extract should be concentrated before analysis. When the hydrocarbon content in the desulfurization solvent exceeds 1000 mg/kg, emulsification may occur in the original solvent sample, and the system may appear as a suspension. In this case, the sample should be thoroughly shaken to ensure homogeneity before extraction. During

phase separation, emulsification may still influence the analytical results. To promote phase separation, the sample can be transferred into a centrifuge tube and centrifuged at 5000 r/min for 3 min. The concentration step is sometimes difficult to control. If the extract volume after concentration is less than 1 mL, n-hexane can be added to adjust the final volume to 1 mL.

4. Conclusions

Based on field samples and the MDEA-based UDS solvent matrix, a quantitative method for determining hydrocarbon impurities in UDS desulfurization solvents was developed through compositional analysis, theoretical calculations, and experimental validation. The results show that hydrocarbon impurities in the desulfurization system of the Western Sichuan gas field are mainly linear alkanes in the C_{13} to C_{18} range. COSMO-RS calculations and intermolecular interaction analysis showed that n-hexane has suitable extraction capacity and selectivity for hydrocarbon impurities in the MDEA-based UDS solvent matrix. Ultraviolet spectrophotometry shows a weak response toward normal alkanes and requires strong acid pretreatment, which disrupts the solvent system and prevents the establishment of a stable linear relationship. The analytical method based on n-hexane extraction coupled with gas chromatography shows good selectivity and sensitivity for hydrocarbons in the C_{10} to C_{20} range. The calibration curve shows good linear correlation with high precision and repeatability. The developed n-hexane extraction-GC method is suitable for the quantitative determination of hydrocarbon impurities in MDEA-based UDS desulfurization solvents. The method provides technical support for hydrocarbon contamination monitoring and solvent management in MDEA-based UDS desulfurization systems. Further matrix-specific calibration is required before extending this method to primary or secondary amine absorbents such as MEA, DEA, and DIPA.

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Abbreviations

The following abbreviations are used in this manuscript:

A	Sample absorbance, %
A_x	Total peak area of the sample, pA·s
b	Slope of the calibration curve
E_{int}	Interaction energy between solvent and solute, kJ/mol
PI^{∞}	Extraction performance index
V	Sample volume, mL
γ_i^{∞}	Activity coefficient at infinite dilution
A_0	Blank absorbance, %

a	Intercept of the calibration curve
C_i^{∞}	Solvent capacity
MPI	Molecular polarity index
S^{∞}	Extraction selectivity at infinite dilution
V_1	Volume of extraction solution, mL
ρ	Hydrocarbon impurity content, mg/kg

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