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ZiYang Zhao

Chinese Academy of Sciences

Xizhe Li

1xz69@petrochina.com.cn

Chinese Academy of Sciences

Ruilan Luo

Research Institute of Petroleum Exploration and Development

Longyi Wang

Chinese Academy of Sciences

Yuchuan Chen

China University of Geosciences (Beijing)

Sijie He

China University of Geosciences (Beijing)

Wenxuan Yu

Research Institute of Petroleum Exploration and Development

Yuhang Zhou

Chinese Academy of Sciences

Zan Huang

Research Institute of Petroleum Exploration and Development

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Molecular dynamics simulation of natural gas drag reducing agents on iron surfaces under the dual-carbon background

ZiYang Zhao^{1,2,3}, Xizhe Li^{1,2,3*}, Ruilan Luo³, Longyi Wang^{1,2,3}, Yuchuan Chen⁵,
Sijie He⁵, Wenxuan Yu³, Yuhang Zhou^{1,2,3} and Zan Huang³

1. School of Engineering Science, University of Chinese Academy of Sciences, Beijing 100049, China

2. Institute of Porous Flow & Fluid Mechanics, Chinese Academy of Sciences, Langfang 065007, China

3. Research Institute of Petroleum Exploration and Development, PetroChina, Beijing 100089, China

4. Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China

5. School of Energy Resource, China University of Geosciences (Beijing), Beijing 100083, China

* Corresponding author: Xizhe Li. School of Engineering Science, University of Chinese Academy of Sciences, Beijing 100049, China, E-mail: lxz69@petrochina.com.cn

Abstract: To address the issues of high energy consumption and significant carbon emission intensity in long-distance natural gas pipelines, a molecular dynamics simulation of natural gas drag-reducing agent adsorption on iron surfaces and a numerical simulation of agent-added transportation were conducted to meet the low-carbon demands of oil and gas surface processes under the dual-carbon strategy. The Materials Studio software was utilized to construct the solid-liquid interface models of the iron atomic layer with three representative drag reducing agents, namely CPA, BIB, and corrosion-inhibiting G10, and the adsorption energies of the drag reducing agent molecules on the Fe surface under different mass fractions were calculated. The ANSYS Fluent software was employed to simulate the flow field characteristics inside the pipeline before and after agent addition, and to analyze the intrinsic correlation among the drag-reducing agent, iron surface adsorption, and macroscopic drag reduction. The results indicate that as the mass fraction of the drag reducing agent increases from 10% to 20%, the adsorption energies of CPA, BIB, and G10 on the Fe atomic layer increase by 53.84%, 26.87%, and 60.98%, respectively. The G10 drag reducing agent, containing siloxane groups, forms Si-O covalent bonds on the iron surface, and its adsorption energy improvement is significantly superior to that of CPA and BIB containing carboxylic acid groups.

After the addition of CPA and G10, the average flow velocity in the pipeline increases from 10.183 m/s to 10.637 m/s and 10.943 m/s, the throughput increases by 12.37% and 14.79%, respectively, and the average turbulence intensity decreases by 37.4% and 59.6%, respectively. The research results provide theoretical support for the molecular structure design of natural gas drag-reducing agents and for energy conservation and emission reduction in pipeline transportation under the dual-carbon target.

Keywords: Dual-carbon target; Natural gas pipeline; Drag reducing agent; Molecular dynamics simulation; Adsorption energy; Low-carbon surface process

0 Introduction

Guided by the "carbon peaking and carbon neutrality" strategy, natural gas acts as a clean and low-carbon bridging energy source and plays a key role in the transformation of China's energy structure. According to statistics from the International Energy Agency, global natural gas consumption reached $4.212 \times 10^{12} \text{ m}^3$ in 2024, representing a year-on-year increase of approximately 2.8%, and accounted for nearly 40% of the new global energy demand^[1]. Domestic natural gas consumption reached $3.945 \times 10^{11} \text{ m}^3$ in 2023, exhibiting a year-on-year increase of 7.6%, and domestic consumption is projected to exceed $6 \times 10^{11} \text{ m}^3$ by 2030. The long-distance pipeline transportation of natural gas is an essential component of oil and gas surface processes, and its energy consumption and compressor emissions directly influence the carbon intensity of the pipeline network. Any reduction in frictional resistance will directly translate into a synchronized decrease in compressor power consumption, fuel gas self-consumption, and CO₂ emissions, which serves as a direct approach to achieving low-carbon surface processes and represents a key starting point for synergistic innovation between oil and gas surface engineering and environmental protection under the dual-carbon background.

Modern long-distance pipelines exhibit a developmental trend toward long distances, large diameters, and high pressures^[2], and the friction loss caused by wall roughness, turbulent dissipation, and internal coating aging constitutes the primary source of pipeline operational energy consumption. Current primary pipeline drag reduction technologies can be classified into two main categories: the first is internal wall coating drag reduction based on surface engineering, which suppresses near-wall turbulence by covering the pipe wall with low surface energy materials to form a microscopically smooth surface; the second is the drag reducing agent addition technology based on flow field regulation, which reconstructs the near-wall flow field through the viscoelastic properties of high-molecular polymers or surfactants injected into the fluid. Internal coating technology has been applied in newly constructed pipelines, but it faces bottlenecks such as complex construction, degradation of drag reduction performance after long-term operation, and difficulties in retrofitting old pipelines, making it difficult to meet the urgent demand for large-scale energy conservation and carbon reduction in pipeline networks under the dual-carbon background. In contrast, injecting high-molecular drag reducing agents into natural gas^[3-6] forms an ordered adsorption film on the pipeline inner wall through polar groups and suppresses turbulent fluctuations in the near-wall region via non-polar segments. This approach can achieve throughput enhancement and energy consumption reduction under low-cost and controllable dosing conditions, and it is not restricted by whether the pipelines are new or old or whether coatings are applied, thus becoming a surface process optimization pathway that possesses both economic and low-carbon benefits^[7].

Since the discovery of the Toms effect in 1948, liquid drag reduction has achieved large-scale application in the field of crude oil transportation. In 1979, the drag reducing agent developed by Conoco in the United States pioneered commercial application in crude oil pipelines, resulting in a 20% to 30% increase in transportation efficiency for the Trans-Alaska Pipeline System after agent addition. The annual global consumption of drag reducing agents for oil pipelines has stabilized at the order of 10^5 tons, and over 90% of main oil pipelines have incorporated drag reducing agents into their regular process configurations^[8-10]. Research on gas drag reduction began relatively late, in 1956, the American Petroleum Institute first reported the possibility of obtaining a 15% to 25% improvement in pressure drop by injecting liquid drag reducing agents into gas pipelines^[11]. The atomized gas drag reduction scheme proposed by Lowther^[12] could achieve a 15% to 35% increase in gas volumetric flow rate while maintaining a constant pressure drop. Naess^[13,14] systematically investigated the applicability of two types of drag reducing agents, film-forming agents and viscoelastic agents, for new and old pipelines as well as internally coated pipelines. Chen et al. field-tested an amine-based corrosion-inhibiting and drag-reducing agent in a subsea gas pipeline in the

Gulf of Mexico, confirming its drag reduction reliability. Domestic researchers including Zhang Jinling, Bao Xuchen, Li Guoping, Xing Wenguo, and Guo Haifeng^[15-17] successively developed series of drag reducing agents such as BIB, CPA, and G10, and summarized three categories of mechanisms: smooth drag reduction, viscoelastic drag reduction, and synergistic drag reduction. The field drag reduction rates are generally between 8% and 22%, and the effective duration of a single injection of the BIB atomized drag reducing agent can reach up to 90 days. However, existing studies mostly focus on macroscopic drag reduction performance and synthesis processes, lacking a systematic understanding of the microscopic adsorption mechanism of drag reducing agent molecules on the pipeline iron inner wall and the quantitative correlation between adsorption energy and macroscopic drag reduction performance. Furthermore, there is a lack of quantitative carbon reduction evaluation oriented toward the dual-carbon strategic target, which limits the molecular design and engineering scale-up of drag reducing agents to a certain extent.

In view of this, taking typical carboxylic acid-type (CPA, BIB) and siloxane-phosphate ester-type (G10) drag reducing agents as research subjects, this paper reveals the variation laws of their adsorption energies on iron surfaces based on molecular dynamics simulations. Through Fluent numerical simulations, the variations in the pipeline flow field, turbulent kinetic energy, and throughput before and after agent addition are quantitatively evaluated to elucidate the intrinsic correlation among "molecular structure, interfacial adsorption, macroscopic drag reduction, and low-carbon benefits". This provides theoretical guidance for the low-carbon transformation of natural gas surface processes and the molecular design of drag reducing agents under the dual-carbon background.

1 Theoretical analysis of drag reduction transportation in natural gas pipelines

1.1 Mechanism of pipeline transportation resistance loss

The pressure loss in natural gas pipelines consists of frictional resistance loss along the pipeline and local resistance loss, where the former is described by the Darcy-Weisbach equation:

$$\Delta p_f = \lambda (L/D) \left(\frac{\rho v^2}{2} \right) \quad (1)$$

where λ is the Darcy friction factor, which correlates with the Reynolds number Re and relative roughness ε/D ; L and D represent the length and internal diameter of the pipeline, respectively, in m; ρ is the density of natural gas, in kg/m^3 ; and v is the flow velocity, in m/s. The Reynolds number for engineering trunk lines generally exceeds 10^6 , falling within the fully rough turbulent flow regime, where the friction factor is determined by the Colebrook-White equation and is primarily governed by the absolute roughness of the pipe wall K ^[18].

Derivations demonstrate that, under conditions of a constant pipe diameter, pipe length, and flow velocity, the pressure drop along the pipeline $\Delta P \propto K^{0.25}$, and the throughput $Q \propto K^{0.125}$. Therefore, reducing the effective roughness of the pipeline internal wall is the key to enhancing throughput and lowering compressor power consumption and carbon emissions. For a typical 1016 mm trunk line, if the absolute wall roughness is reduced from 0.180 mm to 0.060 mm, the theoretical pressure drop can decrease by approximately 24%, accompanied by a synchronized reduction in compressor power consumption and fuel gas self-consumption. The resulting CO_2 emission reduction effect is of significant importance for achieving the dual-carbon target.

1.2 Turbulent drag reduction mechanism of drag reducing agents

Natural gas drag reducing agents are mostly amphiphilic high-molecular polymers containing

a polar head group and a long-chain non-polar tail group, and their molecular structures are similar to organic corrosion inhibitors. The polar groups containing highly electronegative atoms such as N, O, S, and P are adsorbed onto the metal pipe wall through coordination bonds, hydrogen bonds, or covalent bonds, while the non-polar sections composed of C-H chains extend toward the fluid side to form a hydrophobic, low-surface-energy barrier. This structure determines that the drag reducing agent simultaneously possesses dual functions of interfacial regulation and fluid regulation at its polar and non-polar ends. Its drag reduction mechanisms primarily include^[19-22]: (1) smooth drag reduction, where the polar end adsorbs and fills the nano to micro-scale pits and grooves on the pipe wall, reducing the effective roughness to achieve a drag reduction of over 10%;(2) viscoelastic drag reduction, where the non-polar segments form a molecular film layer with an elastic response near the wall, enabling near-wall molecular collisions to become approximately elastic, which absorbs turbulent kinetic energy fluctuations and redistributes about 60% to 75% of it to the mainstream region in the form of thermal energy, thereby delaying the transition from laminar flow to turbulent flow and attenuating turbulence intensity by 30% to 45%;(3) a synergistic effect of the two, where the polar end forms an ordered adsorption layer on the iron surface via van der Waals forces, hydrogen bonds, or covalent bonds, while the non-polar end extends outward to constitute a low-surface-energy barrier, increasing the viscous sublayer thickness by 3 to 5 times and reconstructing the near-wall flow field from the perspective of boundary layer topology. Based on the aforementioned mechanisms, the adsorption strength and stability of the drag reducing agent on the iron surface act as the critical microscopic factors governing macroscopic drag reduction performance, which also serve as the core starting point for molecular dynamics simulation research.

2 Molecular dynamics simulation of natural gas drag reducing agents

2.1 Simulation subjects and modeling methods

Comprehensively considering field application effectiveness and duration^[23-26], three representative natural gas drag reducing agents were selected:① CPA drag reducing agent (carboxylate polymer agent), an organic carboxylic acid polymer synthesized by the reaction of a secondary amine, morpholine, acetaldehyde, and succinic acid, with the R group assigned as an eicosyl group ($-C_{20}H_{41}$);② BIB drag reducing agent, a heterocyclic organic carboxylate polymer synthesized using butanedioic acid instead of succinic acid, where the polar end is dominated by amide and carboxyl groups, and the R group is also assigned as $-C_{20}H_{41}$;③ G10 corrosion-inhibiting drag reducing agent, a six-membered cyclic alkyl siloxane-phosphate ester compound generated by the reaction of a long-chain alkyl phosphate monoester and long-chain alkyl methyl dimethoxysilane, with the R group assigned as $-C_{15}H_{31}$. The three types of drag reducing agents encompass two typical polar head group structures: the carboxylic acid type and the siloxane type, as shown in Table 1.

Table 1 Comparative analysis of drag reduction effects among different natural gas drag reducing agents

Application scenario	Drag reducing agent type	Dosing flow rate/ $L \cdot h^{-1}$	Drag reduction efficiency/%	Effective duration/ d
Shaanxi-Beijing natural gas pipeline	CPA drag reducing agent	76	11.5-15.6	>60
No. 1 Gas Production Plant of Changqing Oilfield	BIB-type drag reducing agent	30-100	8-10	>90
No. 1 Gas Production Plant of Changqing Oilfield	G10 corrosion-inhibiting drag reducing agent	—	28.8	>30

Northwest Oilfield gathering and transportation pipeline	BDMET drag reducing agent	4.17	8~13	>20
Lanzhou-Chengdu-Chongqing refined oil pipeline	KS-30 drag reducing agent	9.20	41.6	<20

The Amorphous Cell module in the Materials Studio software was employed to construct AC boxes of drag reducing agent-CH₄ solutions at two mass fractions of 10% and 20%, respectively; Three Fe atomic layers were constructed as the pipeline inner wall model via cleavage along the Fe(110) plane, and the Layers module was used to combine the AC box with the Fe layers to build a solid-liquid interface model. The Forcite module was utilized, selecting the COMPASS force field for geometric optimization and NVT ensemble dynamics simulation. The temperature was set to 298 K, the time step was 1 fs, and the total simulation time was 200 ps. After energy convergence, the adsorption energy between the drag reducing agent molecular layer and the Fe atomic layer was statistically calculated. The schematic diagram of the simulation is shown in Figure 1 and Figure 2.

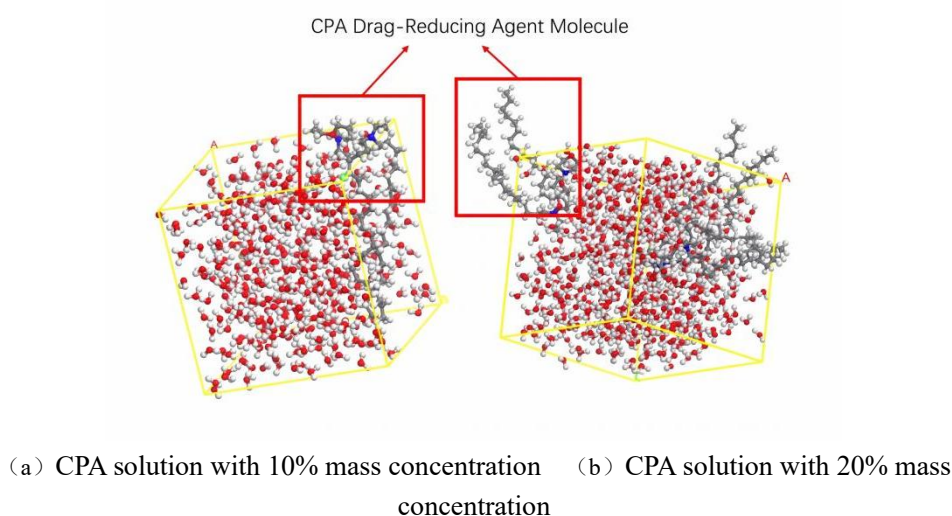


Figure 1 Schematic diagram of AC boxes for CPA drag reducing agent solutions with different concentrations

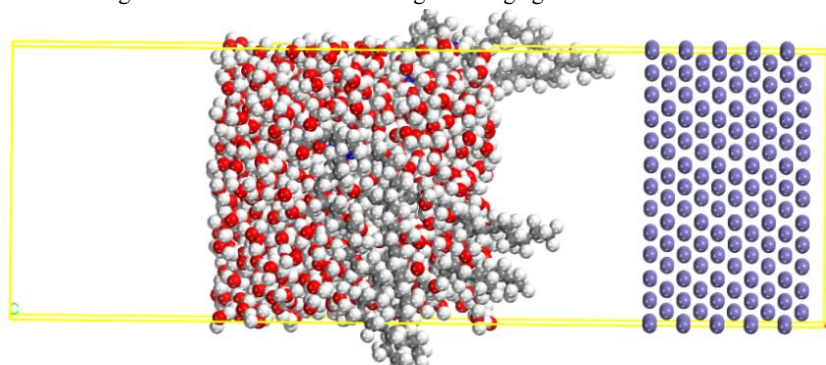


Figure 2 Microscopic schematic diagram of the solid-liquid interface between drag reducing agent molecules and iron atoms

2.2 Simulation results of adsorption energy

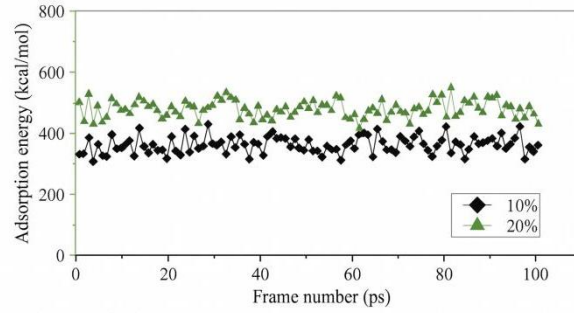
The variations in adsorption energies of the three types of drag reducing agents with the Fe atomic layer under the two mass fractions are shown in Table 2.

Table 2 Comparison of adsorption energies of different categories of natural gas drag reducing agents on the Fe surface

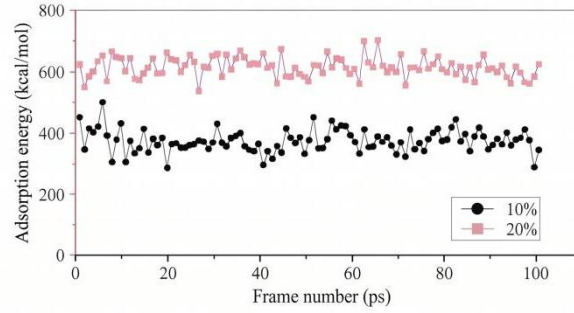
Natural gas drag reducing agent category	Mass fraction concentration $\phi/\%$	Adsorption energy / $\text{kcal} \cdot \text{mol}^{-1}$	Variation magnitude of adsorption energy before and after concentration change
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CPA	10	398.2296	53.84%
	20	612.6539	
BIB	10	385.5586	26.87%
	20	489.1407	
G10	10	475.1522	60.98%
	20	764.9012	

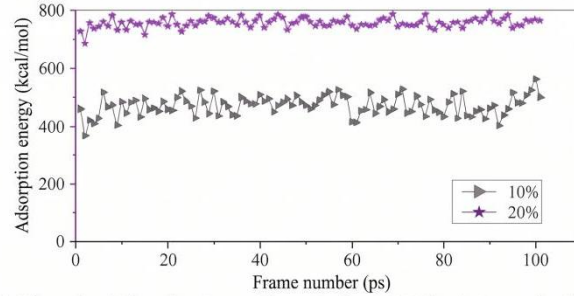
As shown in Table 2: (1) As the mass fraction increases from 10% to 20%, the adsorption energies of all three types of drag reducing agents exhibit a significantly increasing trend, elevating by 53.84%, 26.87%, and 60.98%, respectively. This indicates that appropriately increasing the dosing mass fraction helps to form a denser and more stable adsorption film on the iron pipe wall, thereby enhancing the filling capability for wall unevenness defects and the suppression capability for near-wall turbulent fluctuations. (2) Both the absolute value and the increment of the adsorption energy of the G10 drag reducing agent, which contains siloxane groups, are remarkably higher than those of CPA and BIB. The reason is that CPA and BIB utilize carboxylic acid, amide, or amino groups as polar head groups, which bind to the Fe surface primarily through coordination adsorption and acid-base interactions, and are influenced by local pH and competitive adsorption. Conversely, the siloxane groups in G10 can form numerous Si-O-Fe covalent bonds with exposed oxidation sites on the Fe surface, resulting in stronger adsorption and better stability, thus making it more suitable for trunk pipelines that require long-term, low-carbon operation. (3) The heterocyclic acid salt structure of the BIB molecule may undergo configurational rearrangement due to inter-chain steric hindrance after the concentration is increased, leading to an adsorption energy increment significantly smaller than those of CPA and G10. This suggests that the spatial configurational effects of polar head group density and non-polar chain length should be weighed in subsequent molecular design.



(a) Schematic of Adsorption Energy Change During CPA Molecular Dynamics Simulation



(b) Schematic of Adsorption Energy Change During BIB Molecular Dynamics Simulation



(c) Schematic of Adsorption Energy Change During G10 Molecular Dynamics Simulation

Figure 3 Schematic diagram of adsorption energy variations during the molecular dynamics simulation of the three drag reducing agents

In this section, a molecular dynamics simulation method was utilized to investigate the adsorption process of natural gas drag reducing agents on the metal inner wall surfaces from a microscopic perspective, and the mechanism by which different groups in drag reducing agent molecules exert drag reduction effects was elucidated. This provides beneficial guidance for the molecular design and industrial development of natural gas drag reducing agents; however, the specific drag reduction effects of agent-added natural gas pipeline transportation require further verification through simulation experiments.

3 Simulation evaluation of drag reduction transportation effects in natural gas pipelines with agent addition

3.1 Physical models and computational methods

PRO/E4.0 was employed to construct a straight pipe geometric model with an internal diameter of 32 mm, a wall thickness of 3 mm, and a length of 1.4 m, and AutoCAD was used to draw the roughness profile of the pipeline internal wall containing random asperities. The model was imported into the Gambit software for meshing with triangular unstructured grids, where the near-wall region was refined with boundary layers. The total number of grids was approximately 1.8×10^6 , and the error in the grid independence verification was less than 2%.

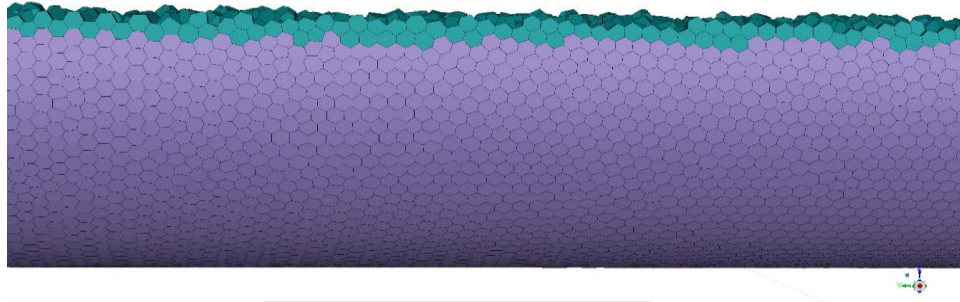


Figure 4 Schematic diagram of the volume mesh for the pipeline internal wall roughness

The governing equations included the continuity equation, momentum equation, energy equation, and SRK equation of state. The RNG k- ϵ model was adopted for turbulence. Compared with the standard k- ϵ model, this model introduces swirl modifications and low-Reynolds-number effect corrections, rendering it more suitable for solving vortex flow fields with rough walls. The solver employed a pressure-based segregated SIMPLE algorithm, and a second-order upwind scheme was applied to the convection terms.

Boundary condition settings: A velocity inlet was used for the inlet with an initial flow velocity of 15 m/s, and turbulence parameters were assigned based on the empirical relationship between the inlet hydraulic diameter and Re; a pressure outlet was used for the outlet with a static pressure of 50 kPa; and a no-slip adiabatic boundary condition was applied to the wall. Based on the adsorption thickness of the drag reducing agent on the iron surface and the actual absolute roughness of the pipe wall, three roughness schemes were established: the original pipeline, the pipeline with CPA addition, and the pipeline with G10 addition, as presented in Table 3.

Table 3 Pipeline roughness schemes

Pipeline type	Absolute roughness K/mm
Original pipeline	0.180
Pipeline with CPA drag reducing agent	0.100
Pipeline with G10 corrosion-inhibiting drag reducing agent	0.060

3.2 Analysis of flow field and drag reduction performance

The velocity distributions and turbulent kinetic energy distributions inside the pipeline under the three working conditions were extracted via CFD-Post, and the main calculation results are presented in Table 4.

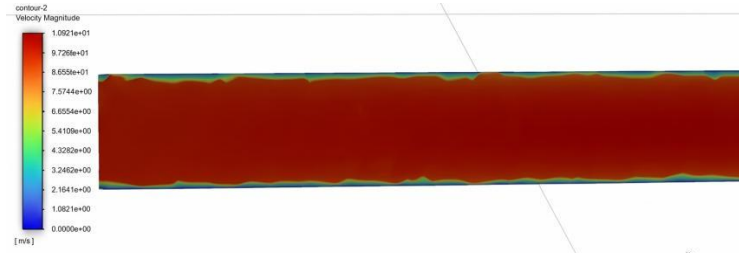
Table 4 Comparison of characteristic parameters of pipeline flow fields before and after agent addition

Pipeline type	Average flow velocity/($\text{m}\cdot\text{s}^{-1}$)	Throughput enhancement/%	Average turbulence intensity
Original pipeline	10.183	—	1.413
With CPA drag reducing agent	10.637	12.37	0.787
With G10 corrosion-inhibiting type	10.943	14.79	0.571

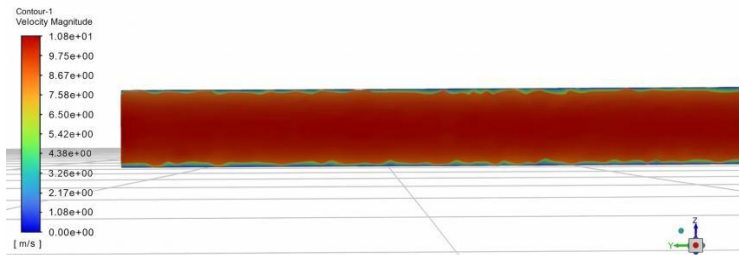
A comparison of the velocity fields indicates that significant flow velocity gradient mutations and velocity deficit regions exist near the protrusions on the internal wall of the original pipeline, which constitute the primary sources of form drag and turbulent dissipation; After adding the drag reducing agents, the roughness decreases, the protrusion heights are effectively reduced, the near-wall flow velocity gradient tends to become gentle, and the axial velocity distribution becomes more uniform. The average flow velocities increase by 4.46% (CPA) and 7.46% (G10), respectively, compared with the original pipeline, corresponding to throughput enhancements of 12.37% and

14.79%.

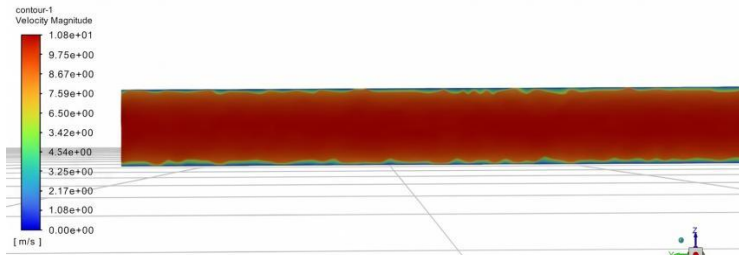
A comparison of the turbulent kinetic energy fields indicates that the turbulent kinetic energy peaks before and after the protrusions in the original pipeline are high and cover a wide range, with the average turbulence intensity reaching 1.413, serving as the main contribution to energy dissipation and friction loss; After agent addition, the internal wall protrusions of the pipeline are weakened, the turbulent kinetic energy peaks decline, and the average turbulence intensities decrease to 0.787 and 0.571, respectively, with reduction rates reaching 37.4% and 59.6%. This demonstrates that the drag reducing agent forms a dense adsorption film on the iron surface to reduce the effective roughness, thereby suppressing near-wall turbulent fluctuations and reducing the transport of wall shear energy by Reynolds stress, which is the core physical mechanism for achieving friction reduction and throughput enhancement.



(a) Velocity contours for original pipeline

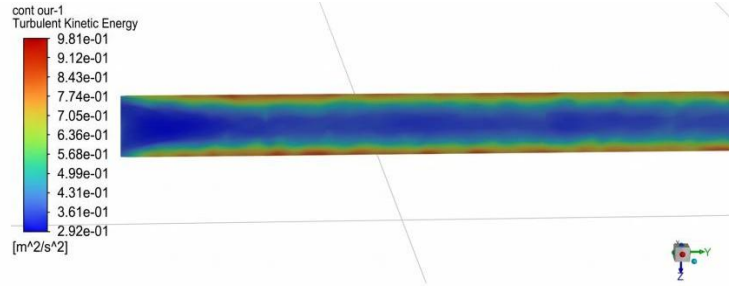


(b) Velocity contours for pipeline with CPA drag-reducing agent

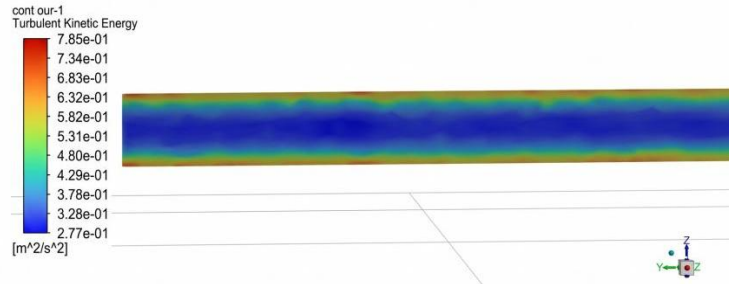


(c) Velocity contours for pipeline with G10 corrosion-inhibiting drag-reducer

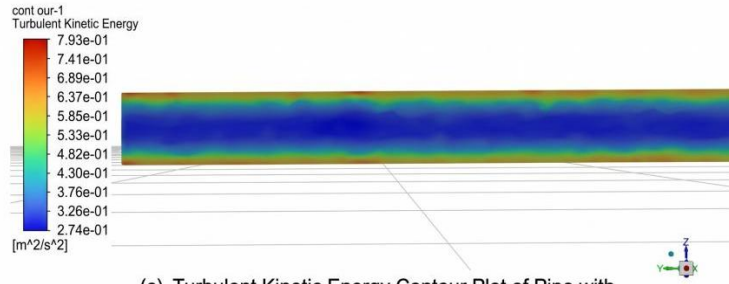
Figure 5 Comparison of pipeline velocity contours before and after agent addition



(a) Turbulent Kinetic Energy Contour Plot of Original Pipe



(b) Turbulent Kinetic Energy Contour Plot of Pipe with Added CPA Drag Reducer



(c) Turbulent Kinetic Energy Contour Plot of Pipe with Added G10 Corrosion-Inhibiting Drag Reducer

Figure 6 Turbulent kinetic energy contour of original pipeline

3.3 Correlation between molecular adsorption and macroscopic drag reduction

Comparing the adsorption energy results in Section 2.2 with the macroscopic drag reduction performance in this section, it is evident that the G10 drag reducing agent possesses the highest adsorption energy on the Fe surface and the largest increment in adsorption energy, which corresponds to the most significant enhancements in pipeline throughput and reductions in turbulence intensity, exhibiting a clear positive correlation. This indicates that the interfacial adsorption strength of the drag reducing agent on the iron pipe wall acts as the microscopic basis governing macroscopic drag reduction performance. By introducing siloxane-based polar groups capable of forming covalent bonds with the Fe surface and moderately increasing the dosing mass fraction, the adsorption stability and drag reduction durability of the drag reducing agent on the pipe wall can be significantly enhanced, providing a quantifiable microscopic criterion for the molecular structure design of drag reducing agents oriented toward the dual-carbon target.

Furthermore, taking a typical trunk line as an example to estimate the low-carbon benefits: for a 1016 mm trunk line with an annual throughput on the order of $1 \times 10^{10} \text{ m}^3$, if the injection of the G10 drag reducing agent reduces friction by approximately 30% and enhances throughput by approximately 15%, the operational load of compressor stations as well as fuel gas and electricity consumption can be proportionally reduced while maintaining the annual throughput target. Estimating that compressor energy consumption accounts for 70% of the pipeline operational energy consumption, the comprehensive energy consumption per kilometer can decrease by approximately 8% to 10%, and the corresponding annual reduction in indirect CO_2 emissions for modern long-

distance pipelines dominated by electric compressors can reach tens of thousands of tons. If synergistic measures such as CCUS/CCS and renewable energy power supply are integrated, the carbon intensity in the long-distance natural gas transportation sector is expected to decline further, which is highly consistent with the low-carbon transformation targets for surface processes in the oil and gas industry under the national "14th Five-Year Plan" and the vision of carbon neutrality by 2060, fully reflecting the value orientation of synergistic innovation between oil and gas surface engineering and ecological environmental protection.

4 Conclusions

This study employed the Materials Studio and Ansys Fluent software to simulate the adsorption effects, drag reduction effects, and drag reduction mechanisms of natural gas drag reducing agents by varying the mass concentration of drag reducing agent molecules, utilizing different categories of natural gas drag reducing agents, and adjusting the pipeline internal wall roughness. The variation laws of adsorption energies for drag reducing agents at different concentrations and the flow velocities before and after roughness alterations were primarily analyzed. The main conclusions are as follows:

(1) Molecular dynamics simulations based on Materials Studio demonstrate that as the drag reducing agent mass fraction increases from 10% to 20%, the adsorption energies of CPA, BIB, and G10 drag reducing agents on the Fe atomic layer increase by 53.84%, 26.87%, and 60.98%, respectively; the G10 drag reducing agent containing siloxane groups forms Si-O-Fe covalent bonds on the iron surface, and both the absolute value and the increment of its adsorption energy are significantly higher than those of CPA and BIB utilizing carboxylic acid/amide as polar head groups.

(2) Fluent numerical simulations based on the RNG k- ϵ model reveal that the average fluid flow velocities in the original pipeline, the pipeline with CPA, and the pipeline with G10 corrosion-inhibiting drag reducing agent are 10.183 m/s, 10.637 m/s, and 10.943 m/s, respectively, representing throughput enhancements of 12.37% and 14.79%, respectively; the average turbulence intensities decrease by 37.4% and 59.6%, respectively. The core mechanism for achieving friction reduction and throughput enhancement is that the drag reducing agent forms a dense adsorption film on the iron surface to reduce the effective roughness and suppress near-wall turbulent fluctuations.

(3) The adsorption energy of the drag reducing agent on the iron surface exhibits a significant positive correlation with macroscopic drag reduction performance, which reveals the intrinsic relationship among molecular structure, interfacial adsorption, and macroscopic drag reduction, thereby providing theoretical guidance for the low-carbon transformation of natural gas surface processes and the molecular design of drag reducing agents under the dual-carbon target. It is recommended that subsequent research should orient toward the actual working conditions of long-distance trunk lines to further conduct coupled simulations of the multicomponent natural gas-drag reducing agent-metal interface and life-cycle carbon emission evaluations, and explore the technological pathways for synergistic innovation between oil and gas surface engineering and environmental protection in combination with CCUS/CCS and new energy power supplies.

Author contributions

Z.Z. and X.L. conceived the research. Z.Z. conducted the molecular dynamics and CFD simulations, analyzed the data, and wrote the main manuscript text. R.L. and Z.Z. contributed to the theoretical mechanism analysis. Y.C. and S.H. assisted in numerical modeling and parameter validation. X.W. and Y.Z. prepared Figures 1–3. Z.Z. and L.W. prepared Figures 4–7. Z.H. and Y.C. supervised the

project. All authors reviewed and approved the manuscript.

Data availability

The datasets generated and analyzed during the current study are not publicly available due to the large volume of raw molecular dynamics simulation trajectory data and the involvement of partial simulation configurations and parameter systems in our research group's follow-up unpublished extended studies, but are available from the corresponding author on reasonable request.

Competing interests

The authors declare no completing interests.

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