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Thermodynamically favorable reactions shape the archaeal community affecting bacterial community assembly in oil reservoirs

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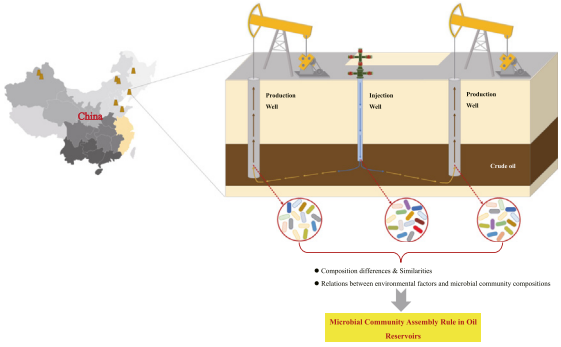
HIGHLIGHTS

- A core microbiota was present in all sampled wells of Chinese oilfield.
- The core bacterial compositions were affected by archaea and abiotic factors.
- The core archaeal community structures were influenced by abiotic factors.
- Thermodynamic constraints were the key for the microbiota assembly in oilfield wells.

GRAPHICAL ABSTRACT



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ABSTRACT

Microbial community assembly mechanisms are pivotal for understanding the ecological functions of microorganisms in biogeochemical cycling in Earth's ecosystems, yet rarely investigated in the context of deep terrestrial ecology. Here, the microbial communities in the production waters collected from water injection wells and oil production wells across eight oil reservoirs throughout northern China were determined and analyzed by proportional distribution analysis and null model analysis. A 'core' microbiota consisting of three bacterial genera, including *Arcobacter*, *Pseudomonas* and *Acinetobacter*, and eight archaeal genera, including *Archaeoglobus*, *Methanobacterium*, *Methanothermobacter*, unclassified *Methanobacteriaceae*, *Methanomethylovorans*, *Methanoculleus*, *Methanosaeta* and *Methanolinea*, was found to be present in all production water samples. Canonical correlation analysis reflected that the core archaea were significantly influenced by temperature and reservoir depth, while the core bacteria were affected by the combined impact of the core archaea and environmental factors. Thermodynamic calculations indicate that bioenergetic constraints are the driving force that governs the enrichment of two core archaeal guilds, aceticlastic methanogens versus hydrogenotrophic

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[1] Jie-Yu Zhao and Bing Hu are co-first authors and contributed equally to this work. As the main focus lies on bioinformatics analysis of the environmental microbial communities, Jie-Yu Zhao is named first.

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Core archaea
Microbiome

methanogens, in low- and high-temperature oil reservoirs, respectively. Collectively, our study indicates that microbial community structures in wells of oil reservoirs are structured by the thermodynamic window of opportunity, through which the core archaeal communities are accommodated directly followed by the deterministic recruiting of core bacterial genera, and then the stochastic selection of some other microbial members from local environments. Our study enhances the understanding of the microbial assembly mechanism in deep terrestrial habitats. Meanwhile, our findings will support the development of functional microbiota used for bioremediation and bioaugmentation in microbial enhanced oil recovery.

1. Introduction

Microorganisms are present in nearly all habitats on the earth and play fundamental roles in global biogeochemical cycles, thus shaping the entire environment of the planet (Bertrand et al., 2015). Community assembly mechanisms are essential for understanding the ecological functions of microorganisms in biogeochemical cycling in Earth's ecosystems (Green et al., 2008; Stearns et al., 2011; Tedersoo et al., 2014). Both deterministic and stochastic processes play important roles in community assembly (Caruso et al., 2011; Stegen et al., 2012). The deterministic processes involve niche-based mechanisms, including microbial interactions and environmental filtering, while the stochastic processes include random births, deaths, colonization, extinction, and speciation (Zhou et al., 2014). However, how these two processes shape the microbial community together is still unclear.

The functional microbial structures of communities are shaped by physical-chemical factors (Louca et al., 2016) and can be explained based on the general laws of thermodynamics and stoichiometry (Delattre et al., 2019). For example, methanogenic archaea play essential roles in hydrocarbon degradation in oil reservoirs by removing products generated in the upstream acidogenic and acetogenic reactions that would otherwise become thermodynamically unfavorable (Leng et al., 2018). Acetotrophic methanogens rather than hydrogenotrophic methanogens were predominant in the anaerobic microbial communities under high caron dioxide (CO_2) partial pressure, because aceticlastic methanogenesis was thermodynamically easier than the syntrophic acetate oxidation linked with hydrogenotrophic methanogenesis under this condition (Mayumi et al., 2013). However, it is still unknown what the basic force is to build up microbial communities in nature and how it drives the assembly of microbial communities.

Modeling the intrinsic mechanism of microbial community assembly in complex natural ecosystems such as soils and oceans, with their multilevel, multifactor, and multivariable characteristics, is a considerable challenge. The use of petroleum reservoirs as object to learn about the microbial community assembly mechanism seems to have potential. Firstly, microbial ecosystems in petroleum reservoirs are seldomly influenced by exogenous abiotic and biotic variables due to their space independence, making them an important type of natural ecosystems on the earth. Secondly, the carbon sources available to microorganisms in petroleum reservoirs were limited to hydrocarbons with different molecular weights, making the microbial members in the ecosystems either oil degraders or companions of oil degraders involved in hydrocarbon mineralization to methane (CH_4) and CO_2 (Head et al., 2003; Jones et al., 2008). The microbiota compositions in petroleum reservoirs have been investigated in Asia, Europe, Africa, North America, and South America (Kotlar et al., 2011; Lenchi et al., 2013; Tang et al., 2012; Yamane et al., 2011). For example, Shelton et al. took production water samples from 22 oil production wells in north central Lousiana, USA, and found that the microbial diversities were driven by the relative extent of crude oil biodegradation, salinity and well depth, but implied that no single member could be the indicator to reflect the crude oil methanogenic capability of the endogenous microbiota (Shelton et al., 2016). Kim et al. expected to develop microbial-enhanced oil recovery strategy for high-temperature oil reservoirs, so they determined the microbial compositions in produced water samples taken from five geographically distant thermophilic oil reservoirs in USA and Canada (70–90 °C), and found that the microbial community structures exhibited high similarity, regardless of the geographical distances or different physiochemical properties in each site (Kim et al., 2018). Sierra-Garcia et al. compared the microbiomes of crude oil and produced water samples taken from high-temperature, relative saline oil wells in Miranga oilfield, Brazil, with and without water flooding, and found that the conventional water flooding elevated the relative proportion of bacteria, introduced a greater metabolic versatility, and changed the in-situ hydrocarbon degradation from anaerobic digestion to aerobic pathways (Sierra-Garcia et al., n.d.). However, most previous microbial ecology studies focused on small amounts of petroleum reservoirs with special properties. The lack of a comprehensive understanding of the microbiota in different petroleum reservoirs interferes with the determination of the pattern of microbiota composition.

Here, we sampled production and injection water samples from different petroleum reservoirs with various geochemical conditions in China and analyzed their microbial compositions using high-throughput 454 pyrosequencing of 16S rRNA genes. Our results show that some core bacterial and archaeal species were universally existent in all samples regardless of the spatial distances, while some other members were locally unique, and that the functional archaeal distribution was in accord with rational thermodynamic constraints, indicating that both deterministic and stochastic processes occurred during the microbial community assembly and that the intrinsic assembly mechanism likely leads toward a thermodynamic window of opportunity.

2. Results

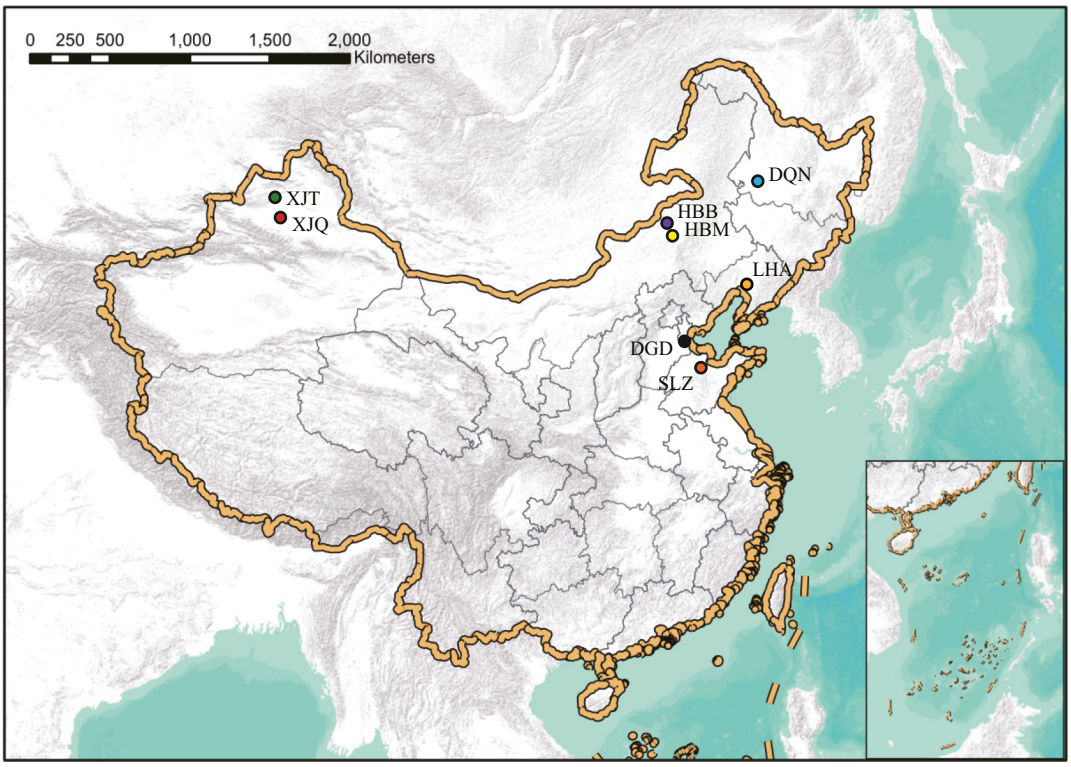
2.1. Spatial variations in physical and geochemical conditions in petroleum reservoirs

In this study, a total of 50 water samples were collected for microbial community analysis from eight injection wells and 42 production wells in eight blocks of various oilfields in northern China, including Dagang Oilfield Block Yangerzhuang (DGD), Daqing Oilfield Northern Block II (DQN), Huabei Oilfield Block Menggulin (HBM) and Block XIX (HBB), Liaohe Oilfield Block A12 (LHA), Shengli Oilfield Block Zhan III (SLZ), and Xinjiang Oilfield Block VI (XJT) and Block VII (XJQ). The locations of the eight oilfields and the geochemical conditions in each water-flooded petroleum reservoir at the sampling time are shown in Fig. 1.

Principal component analysis (PCA) based on environmental parameters showed that geochemical conditions in petroleum reservoirs varied along with spatial variations (Fig. S1). For instance, the geochemical conditions of XJT and XJQ in Northwest China were significantly different from those of DGD and SLZ in North China. Furthermore, Spearman's rank correlation test showed that temperature and depth exhibited a significantly positive correlation ($\rho = 0.851$, $P = 3.444e^{-15}$), while TOC and pH showed a significantly negative correlation ($\rho = -0.807$, $P = 9.8e^{-09}$) (Table S1).

2.2. The composition of the microbial communities varies geographically

Pyrosequencing analysis of the microbial communities in the 50 water samples identified 246,497 and 144,194 bacterial and archaeal sequences, respectively. These sequences were arranged into 6174



Oil Field		XJT	XJQ	DGD	SLZ	DQN	HBB	HBM	LHA
Injection Well		T1	QI	DI	ZI	NI	BI	MI	AI
Production Well		TP1, TP2, TP3, TP4	QP1, QP2, QP3, QP4, QP5	DP1, DP2, DP3, DP4	ZP1, ZP2, ZP3, ZP4, ZP5, ZP6	NP1, NP2, NP3, NP4	BP1, BP2, BP3, BP4, BP5, BP6, BP7	MP1, MP2, MP3, MP4, MP5, MP6, MP7	AP1, AP2, AP3, AP4, AP5
Abiotic Characteristics*	PER (md)	472.14	277.61	3795.34	911.86	2006.08	699.09	688.96	628.17
	POR	0.21	0.17	0.33	0.3	0.3	0.19	0.22	0.21
	Temperature (°C)	20.6	32	58	60	44.6	58.4	37	70
	Depth (m)	480~515	1088	1563.3~1632	120~1360	1155~1207	1446~1539	790~830	1652~2176
	Flooding years (y)	⩾40	⩾39	⩾40	⩾21	⩾50	⩾13	⩾25	⩾19
	WC	0.9	0.62~0.92	0.96	0.9	0.93	0.89	0.92	0.82~0.99
	TSD (mg/L)	5030.96±818.64	5126.30±914.71	3756.12±914.71	6910.00±599.48	1956.80±231.00	1468.36±120.56	1126.07±163.46	999.45±84.29
	TOC (mg/L)	74.24±22.00	40.55±9.37	40.55±9.37	98.76±41.27	97.76±16.62	112.18±35.74	91.86±33.47	6657.00±1539.60
	pH	8.22±0.35	8.26±0.19	7.97±0.22	7.98±0.33	8.03±0.24	8.77±0.38	8.38±0.18	7.50±0.01
	S (%)	0.14±0.06	0.06±0.01	0.28±0.01	2.82±0.20	0.11±0.01	0.18±0.03	0.19±0.01	0.05±0.01
	NI (%)	0.24±0.07	0.18±0.01	0.28±0.02	0.54±0.11	0.15±0.01	0.17±0.01	0.38±0.01	0.08±0.01
	SH (%)	65.46±4.55	61.87±4.88	39.30±2.73	28.23±11.99	46.22±0.17	44.25±0.46	38.94±0.81	45.60±0.87
	AH (%)	15.53±3.90	15.89±2.33	31.85±0.20	34.48±5.14	16.80±1.07	27.86±0.34	17.77±3.99	5.45±2.54
	NH (%)	13.87±3.23	17.49±6.15	22.71±3.98	24.40±6.72	25.60±0.18	16.48±1.26	24.47±1.10	14.06±2.06
	ASP (%)	5.14±2.77	4.76±1.05	6.15±1.05	12.89±0.80	11.39±1.05	11.42±1.38	18.83±3.71	34.90±.040

*PER: Permeability; POR: Porosity; WC: Water content; TSD: Total salinity degree; TOC: Total organic carbon; S: Sulfur; N: Nitrogen; SH: Saturated hydrocarbon; AH: Aromatic hydrocarbon; NH: Non-hydrocarbon; SAP: Asphaltene.

Fig. 1. Geographical distribution of eight oil reservoir blocks in China according to ArcGIS. Fifty water samples from 8 injection wells and 42 production wells were obtained from eight Chinese oilfields (XJT, XJQ, HBM, DQN, DGD, HBB, SLZ, and LHA). The names of the samples taken from the injection and production wells, as well as the physical and geochemical conditions of samples from each oilfield are listed under the map. * PER, Permeability; POR, Porosity; WC, Water content; TSD, Total salinity degree; TOC, Total organic carbon; S, Sulfur; N, Nitrogen; SH, Saturated hydrocarbon; AH, Aromatic hydrocarbon; NH, Non-hydrocarbon; SAP, Asphaltene.

bacterial and 1727 archaeal OTUs. Good's coverage indices for most samples were found to be over 90% (Table S2). Remarkably, the bacterial communities exhibited higher alpha diversity than the archaeal communities, as indicated by the Shannon-Weiner and Simpson indices ($P = 1.391 \times 10^{-6}$ and $P = 4.514 \times 10^{-6}$, Table S2).

Taxonomically, the microbial community structures at the phylum level were similar in different petroleum reservoirs. *Proteobacteria* (45.41–100%) and *Euryarchaeota* (69.93–100%) were the most abundant bacterial and archaeal phyla, respectively, across all samples, and *Bacteroidetes*, *Actinobacteria*, *Firmicutes*, *Caldiserica*, *Crenarchaeota*, and *Thaumarchaeota* were detected in most of the petroleum reservoirs (Fig. S2). However, predominance at the class level varied geographically. *Epsilonproteobacteria* and *Methanomicrobia* were dominant in XJT, DQN, and several HBM production wells, while *Gammaproteobacteria* and *Methanobacteria* were dominant in XJQ, DGD, and HBB, and *Alphaproteobacteria* was only predominant in LHA (Fig. S2).

2.3. Core archaea as the fundamental participants in the microbial communities of petroleum reservoirs

As shown in Fig. 2a and b, based on their frequencies to be identified in injection and production samples of DGD, the archaeal and bacterial

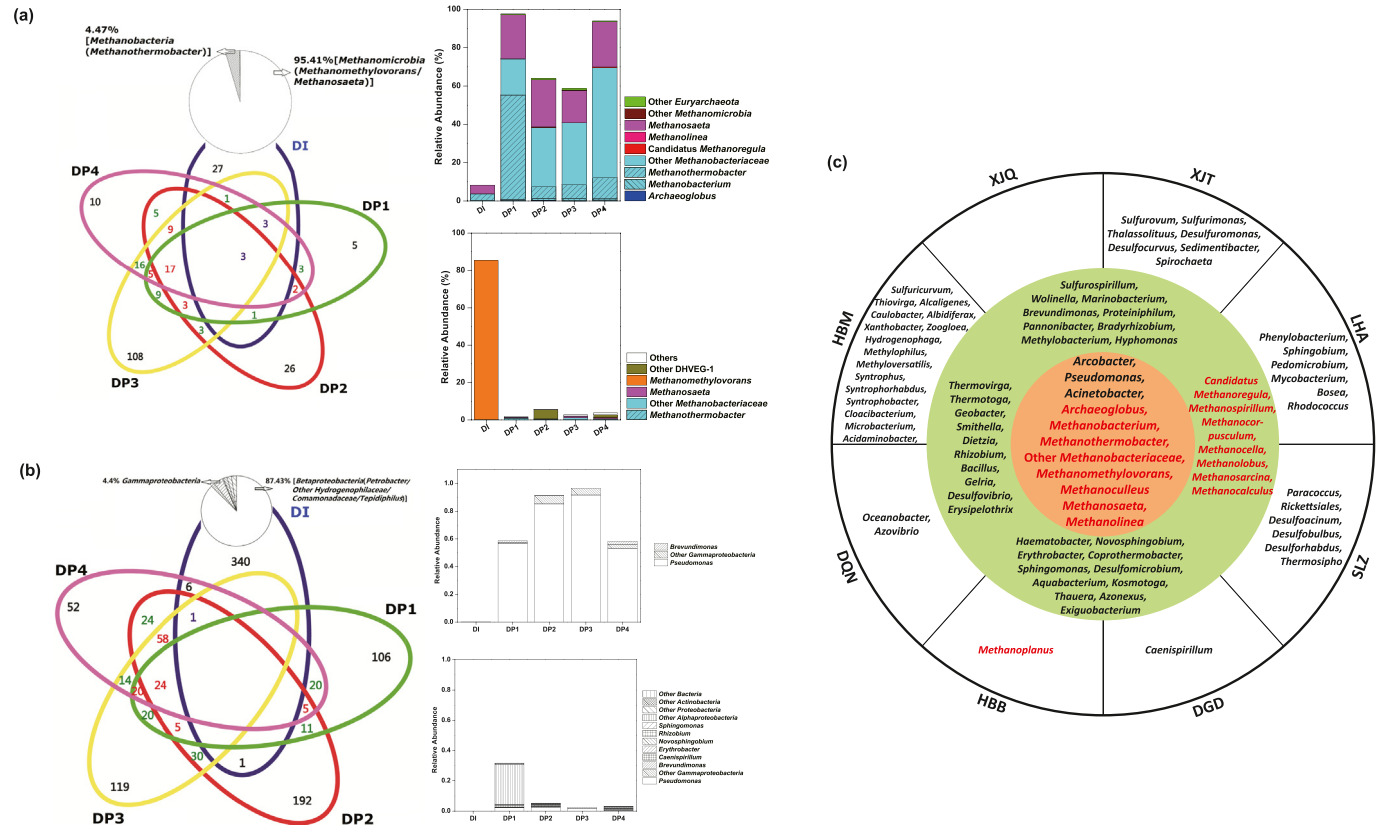


Fig. 2. Identification of the core microbial communities in Chinese petroleum reservoirs. (a) Venn diagram showing the amounts of block-level common and unique bacterial $OTU_{0.03}$ between the injection and production water samples in the DGD block, the pie diagram showing the bacterial composition of injection water, and histograms showing the relative abundances of the core (top) and variable (bottom) bacterial genera in the DGD block. (b) Venn diagram showing the amounts of block-level common and unique archaeal $OTU_{0.03}$ of samples collected from DGD, the pie diagram showing the archaeal composition of injection water, and histograms showing the relative abundances of the core (top) and variable (bottom) archaeal genera in DGD. (c) Core microbial communities in eight Chinese petroleum reservoirs, in which the core bacteria are indicated in pink, variable bacteria in green, and unique bacteria in white (black font), while archaea are indicated in red font in different petroleum reservoirs.

OTUs were grouped into block-level core microbes (OTUs or genera present in >70% of the samples in one block), block-level variable microbes (OTUs or genera present in at least two but <70% of the samples in one block), and block-level unique microbes (OTUs or genera only present in a unique sample). Similar processes were operated on the archaeal and bacterial communities of samples collected from the other seven oilfields to obtain their block-level core, variable and unique microbes (Fig. S3). The block-level core and variable microbes showed greater relative abundances than the block-level unique microbes in every oil reservoir (Table S3). The average proportions of the block-level core and variable microbes at the OUT level and the genus level for all blocks were over 72.19% and 88.26%, respectively. As summarized in Fig. 2c, some block-level core bacterial genera, including *Pseudomonas*, *Acinetobacter*, and *Arcobacter*, and some block-level archaeal genera, including *Archaeoglobus*, *Methanobacterium*, *Methanothermobacter*, unclassified genera affiliated with *Methanobacteriaceae*, *Methanoculleus*, *Methanolinea*, and *Methanosaeta*, were existent in all of the eight blocks, and they were classed as the 'core microbial genera' in the study. The analysis of the relative abundances of core bacterial and archaeal genera in all blocks showed that *Pseudomonas*, unclassified *Methanobacteriaceae*, and *Methanothermobacter* were dominant in XJQ, DGD, and HBB blocks, where the temperature at the sampling sites was moderate-to-high. In contrast, *Arcobacter*, *Methanobacterium*, *Methanosaeta*, *Methanoculleus*, and *Methanolinea* were predominant in XJT, HBM, and DQN blocks, where the temperature was low-to-moderate (Fig. S3). These results indicated that environmental variables should have tight relationship with the core microbial communities in the oilfield blocks.

2.4. Abiotic and biotic factors gradually and consistently shape the microbiota

To evaluate the interactions between the oilfield-derived microbial communities and the abiotic and biotic factors, we conducted canonical correlation analysis (CCA). For the analysis, the core bacterial and archaeal genera were setup as the key biotic factors based on their high relative abundances in all samples. As shown in Table S4, temperature, depth, TOC, pH, AH, and ASP significantly influenced the microbial community structures ($P < 0.05$), four core archaeal genera (*Archaeoglobus*, *Methanothermobacter*, unclassified *Methanobacteriaceae*, and *Methanosaeta*) significantly influenced the bacterial microbial community structures ($P < 0.05$), while no core bacterial genera showed a significant influence on the archaeal communities.

When we compared the explanation degrees of abiotic and biotic variables to the bacterial and archaeal communities using both total and constrained variance, it was found that only 38% of the bacterial community was explained by abiotic factors, while 58% of the archaeal community was explained by abiotic factors. Moreover, the core archaeal genera explained 32% of the bacterial community, while the core bacterial genera explained only 17% of the archaeal community. The integration of abiotic and biotic influences showed that 67% of the bacterial communities were influenced by the integrated factors, which was much higher than the explanation degrees of either abiotic or biotic variables. In contrast to the bacterial communities, the explanation degrees of the integrated factors to the archaeal communities were

similar with those of the individual abiotic variables (Fig. S4). These results indicated that archaeal community structures should be mainly determined by the abiotic variables in petroleum reservoirs, while the bacterial communities were influenced by the integrated abiotic variables and the core archaeal genera.

To analyze association between the abiotic or biotic variables and the abundances of microbial members in the water samples, Spearman's correlation coefficients were calculated and visualized in Fig. 3. It was found that abiotic factors, especially temperature and depth, showed close connections with the surrounding core archaea and provided favorable conditions for the growth of various microbes, indicating that the abiotic factors of temperature and depth and the biotic factors of core archaeal microbiota were the key nodes in the microbial communities of oil reservoirs. In the four blocks with low-to-moderate temperatures (XJT, XJQ, HBM, and DQN), the core archaeal genera with relatively high abundances, including *Methanosaeta*, *Methanolinea*, *Methanoculleus*, and *Methanobacterium*, were negatively correlated with temperature and depth. In the four blocks with moderate-to-high temperatures (DGD, HBB, SLZ, and LHA), the core archaea being predominant in the core microbiota, including

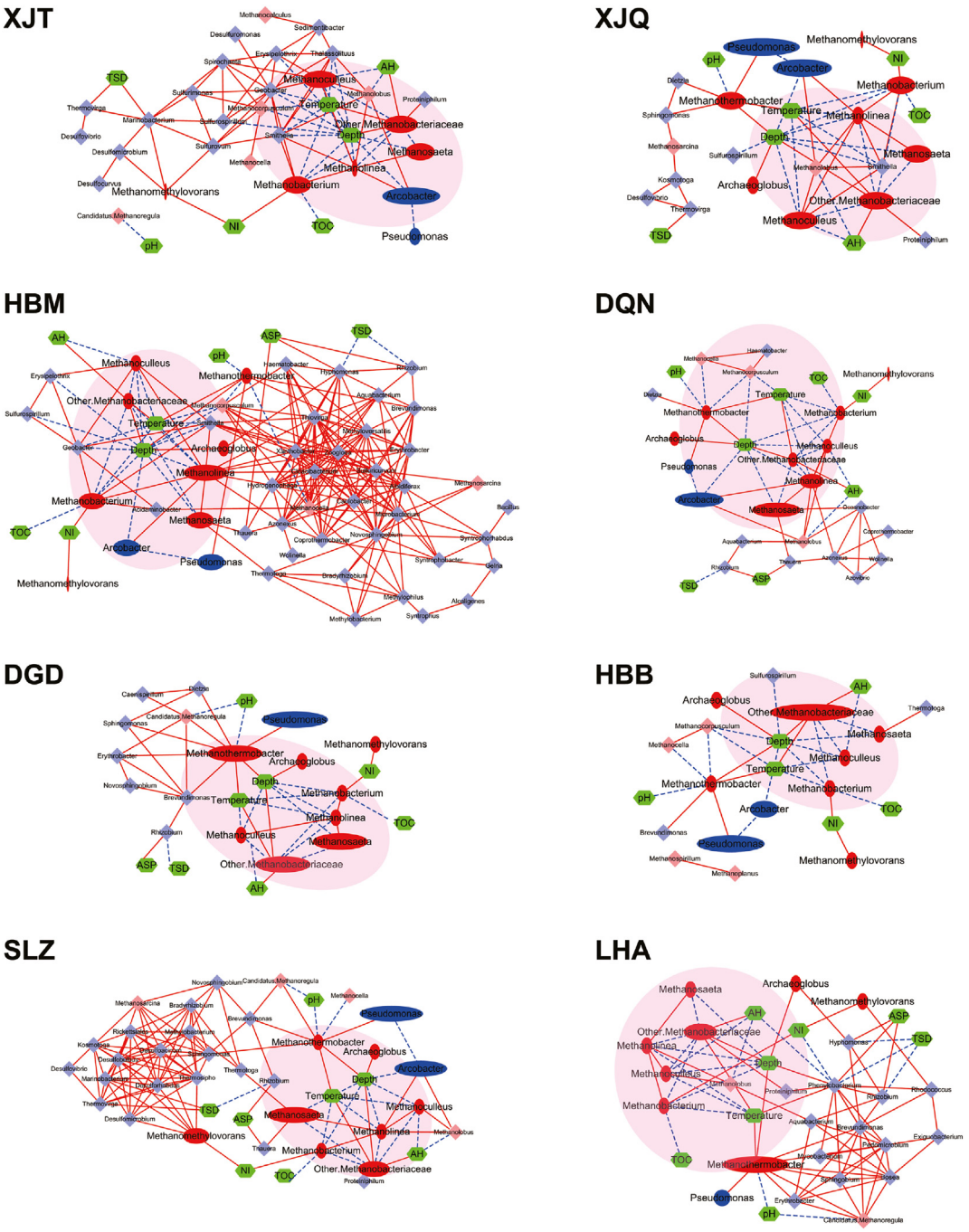


Fig. 3. Network of interactions based on Spearman's rank correlation test ($P < 0.05$, $|\rho| \geq 0.4$), among the core-variable genera in each block and under the indicated geochemical conditions. The nodes represent the geochemical conditions (green), core archaea (red), variable archaea (pink), core bacteria (blue), and variable bacteria (lavender). Only core bacteria and core archaea were present in relative abundance. The path lines correspond to a strong and significant correlation between nodes ($P < 0.05$), shown by positive (red solid line) and negative (blue dashed line) correlations, regardless of connectivity (ρ).

Methanothermobacter and unclassified *Methanobacteriaceae*, showed positively correlated with temperature and depth. For the remaining microbes in the correlation networks, they were directly or indirectly connected with temperature, depth, and the core archaea. For example, in XJT and HBM, the variable bacterial genera of *Geobacter*, *Smithella*, *Arcobacter*, *Hydrogenophaga*, *Azonexus*, *Thauera*, and *Erysipelothrix* showed significantly positive correlations with the core archaeal genera of *Methanoculleus*, *Methanolinea*, *Methanobacterium*, and *Methanosaeta*; In DGD, SLZ and LHA, the core bacterial genus of *Pseudomonas* and the variable bacterial genera of *Brevundimonas*, *Sphingomonas*, and *Sphingobium* showed significantly positive correlations with the presence of *Methanothermobacter*. These findings directed our exploration of the mechanism responsible for microbial community assembly in petroleum reservoirs.

2.5. Deterministic processes influence microbial community assembly in petroleum reservoirs

We analyzed the microbial community structure dissimilarities of water samples derived from different blocks using Bray-Curtis and Jaccard distances. As shown in Table S5, the compositions of the microbiota in the same block were more similar than those identified in different blocks, indicating that different blocks contained microbes that were specifically adapted to those blocks. We next conducted a null model analysis to assess whether the microbiota assembly was characterized by a deterministic or a stochastic process. The permutational analysis of multivariate dispersions (PERMDISP) showed that the observed bacterial and archaeal β-diversities in each of the eight blocks were significantly different from the null random expectations ($P < 0.05$), suggesting that microbial community assemblage in the sampled petroleum reservoirs should be in a deterministic manner (Table S6). To measure the importance of deterministic processes for the assembly of archaeal and bacterial communities in petroleum reservoirs, we then analyzed the proportions of the deterministic processes to the archaeal and bacterial communities, respectively. As shown in Fig. 4, the archaeal communities exhibited higher proportions of deterministic processes (97.08 ± 6.70%) than the bacterial communities (78.75 ± 18.45%). The results indicated that abiotic factors exert a greater influence on the archaeal communities of petroleum reservoirs than the bacterial communities, which was in accordance with the CCA analysis results in Fig. S4.

2.6. Thermodynamic constraints on core archaeal microbiota

To determine the underlying mechanism by which the abiotic factors, such as temperature and depth, influence the archaeal communities and then the bacterial communities in the sampled petroleum reservoirs, the thermodynamic constraints of methanogenic hydrocarbon degradation within the Archaea domain under various temperatures were calculated. The initial substrates of the microbial communities in oil reservoirs are the hydrocarbons. They are ultimately converted to methane (CH_4) through syntrophic associations between bacteria and archaea under the anoxic condition. Firstly, hydrocarbons are degraded to acetate and other short-chain volatile fatty acids by the fermenting bacteria through the hydrocarbon oxidation. Subsequently, acetate is converted to CH_4 either by consortia of acetate-oxidizing bacteria (AOB) and hydrogenotrophic methanogens (HMA) through the syntrophic acetate oxidation linked to hydrogenotrophic methanogenesis or by aceticlastic methanogens (AMA) through the directly aceticlastic methanogenesis (Fig. 5a). As shown in Fig. 5b, the reactions performed by hydrogenotrphic and aceticlastic methanogens were both theoretically exergonic ($\Delta G < 0$) under standard conditions at all temperatures, while the hydrocarbon complete oxidation to produce CO_2 and H_2, the incomplete oxidation to produce acetate and H_2, and the acetate oxidation to CO_2 and H_2 were all energetically unfavorable ($\Delta G > 0$) during the mesophilic and thermophilic digestion of

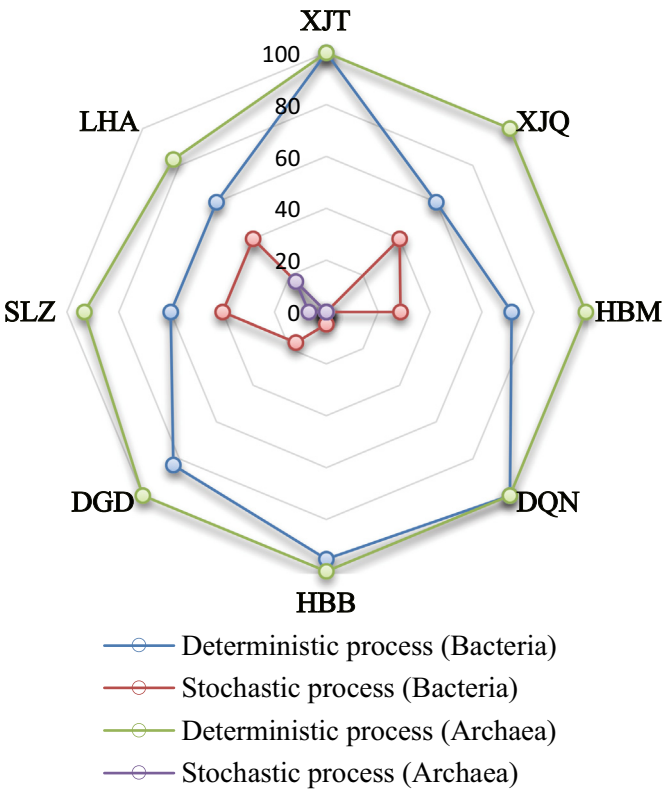


Fig. 4. Proportions of deterministic and stochastic processes of bacterial and archaeal communities in eight blocks.

various hydrocarbons, such as hexadecane ($C_{16}H_{34}$), hectane ($C_{100}H_{202}$) and benzene (C_6H_6). This suggested that the fermenting bacteria in petroleum reservoirs cannot be grown on hydrocarbons in the absence of methanogens. Compared with that in the mesophilic anaerobic digestion, H_2 diffusion efficiency from AOB to HMA was expected to increase, and acetate oxidation by AOB was thermodynamically more favorable in the thermophilic process and at low H_2 partial pressure (Fig. 5c). Therefore, it was considered that methane production through the syntrophic acetate oxidation was more activity at high temperature. This inference was in agreement with the fact that the relative abundances of HMA listed in the core microbiota from our 50 samples of the eight blocks, including the archaeal genera of *Methanobacterium*, *Methanothermobacter*, unclassified *Methanobacteriaceae, Methanoculleus,* and *Methanolinea*, exhibited a significant positive correlation with temperature, whereas the relative abundances of AMA, mainly *Methanosaeta* spp., exhibited a significantly negative correlation with temperature (Fig. 5d). Thus, it was considered that the abiotic factors determined the archaeal community structures in petroleum reservoirs by the thermodynamic constraint-derived recruitment of the core archaeal strains whose metabolism were thermodynamically favorable under special conditions.

3. Discussion

3.1. Abiotic factors drive core archaeal microbiota in petroleum reservoirs

The wells in oil reservoirs are essentially closed and harbor anoxic niches in which the major organic substrates are hydrocarbons. Microbes growing in such reservoirs should predominantly thrive on anaerobic hydrocarbon digestion, in which hydrocarbons are converted to acetate and H_2 and ultimately to biogas composed of CH_4 and CO_2. Since anaerobic hydrocarbon degradation is less exergonic than its aerobic mineralization (Schink, 1997), the bacterial and archaeal microbes

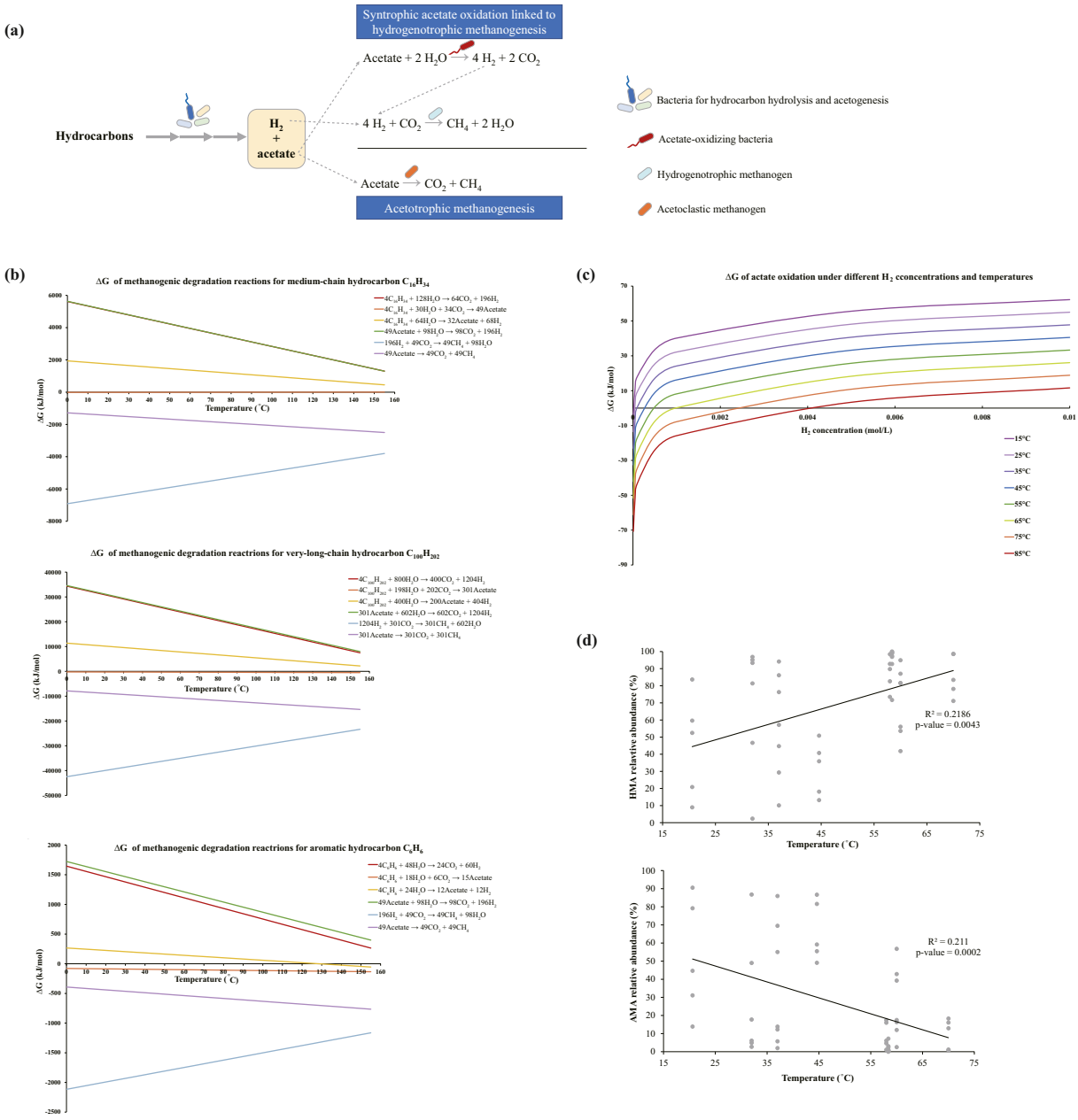


Fig. 5. Thermodynamics of hydrocarbon anaerobic digestion by the oil reservoir-derived microbial communities. (a) The conceptual framework showing the bioprocessing from hydrocarbon to methane (CH_4) under the anoxic condition; (b) The standard molar changes in Gibbs free energy (ΔG) in hydrocarbons (hexadecane, $C_{16}H_{34}$; heactane, $C_{100}H_{202}$; benzene, C_6H_6) complete and incomplete oxidation, acetate oxidation, hydrogenotrophic methanogenesis, and acetotrophic methanogenesis under a temperature range of 0–160 °C at pH 8; (c) ΔG of acetate oxidation under different H_2 concentrations and temperatures; (d) Relationships between the relative abundances of hydrogenotrophic or aceticlastic methanogens (HMA or AMA) and temperature. HMA representing *Methanothermobacter*, other *Methanobacteriaceae*, *Methanolinea*, *Methanoculleus* and *Methanobacterium*; AMAs representing *Methanosaeta*.

in oil reservoirs generally have very close and efficient interactions. Previously, it was considered that the amount of energy released from either the reaction of 'acetate → CO_2 + CH_4' or the reaction of 'H_2+CO_2 → CH_4 + H_2O' was insufficient to feed two microbes, and that the former reaction could only support the growth of AMA while the later one could feed HMA alone (Zeikus, 1977). But the finding of several acetate-oxidizing bacteria in recent decades demonstrated that the former reaction could be achieved through the efficient cooperation of AOB and HMA (Gieg et al., 2014). Schink suggested that the higher the temperature, the more exclusively the syntrophic acetate oxidation coupled with hydrogenotrophic methanogenesis could operate according to his thermodynamic calculation (Pasalari et al., 2020). AMA should thermodynamically outcompete HMA in the same niche regardless of the temperature, because the free energy change goes to AMA from aceticlastic methanogenesis is equal to that shared by the syntrophs of AOB and HMA through the syntrophic acetate oxidation. However, HMA are more often observed in extreme conditions compared to AMA (Pasalari et al., 2020). AMA did operate at high temperature in some cases (Tang et al., 2012; Dyksma et al., 2020; Mayumi et al., 2011; Grabowski et al., 2005), while HMA dominated at low temperature in some other cases (Tang et al., 2012; Kryachko et al., 2012; Sakai et al., 2012; Mori and Harayama, 2011), but there is no systematic evidence showing to what extent temperature affects the occurrence of AMA and HMA in the same habitat. Here, we took water samples from 50 wells in eight oilfields throughout northern China, and measured the abiotic conditions and the microbial community compositions. By doing systematic analyses, it was found that the core AMA in the microbiota of Chinese petroleum reservoirs had a relatively high abundance

at low-to-moderate temperatures and were negatively correlated with temperature, while the core HMA showed the opposite trend (Fig. 5d). The Spearman's rank correlation testing and the null model analysis proved that the core methanogenic community compositions were predominantly influenced by the abiotic factors of temperature and depth, and the core bacterial community structures were determined by the core methanogenic communities coupled with the geochemical factors (temperature, depth, TOC, pH, AH, and ASP) (Figs. 3 and 4). As far as we know, this is the first report showing the relationship between temperature and different types of methanogens in the same microbiota systematically.

3.2. Microbial correlations contribute to complex microbial networks

In this study, the null model analysis showed that microbial community assembly was shaped by deterministic factors, including geochemical conditions and species interactions. Abiotic factors and core archaea sustain the network of microbiota in petroleum reservoirs.

In petroleum reservoirs, microbial members may form syntrophic relationships, in which organisms positively, neutrally, or negatively affect their partners, either by direct contact or by the cross-feeding of metabolites, resulting in mutualistic, commensal, or parasitical interactions (Morris et al., 2013; Little et al., 2008). Previous studies have shown that *Pseudomonas*, *Brevundimonas*, *Sphingomonas*, *Sphingobium*, *Hydrogenophaga*, and *Thauera,* which are hydrocarbon-oxidizing microorganisms, initiate hydrocarbon degradation in petroleum reservoirs (van Beilen and Funhoff, 2007). After the initial oxidation, subsequent products such as alcohols, aldehydes, and fatty acids are excreted into the surrounding environment, affecting other microbes. Subsequently, fermentative bacteria (such as *Geobacter* and *Smithella*) take up and reduce compounds such as amino acids, sugars, long-chain fatty acids, lactate, butyrate, and propionate for the production of H_2, CO_2, and acetate. Methanogens (such as *Methanobacterium*, *Methanothermobacter*, *Methanolinea*, and *Methanosaeta*) then take up H_2, CO_2, acetate, and other small organic acids, resulting in the production of CH_4 (Muyzer and Stams, 2008). Second, numerous microbial species may play similar roles in a single petroleum reservoir because crude oil is an important source of abundant carbon compounds. Our results showed that *Thauera*, *Azonexus*, *Zoogloea*, and *Hydrogenophaga*, affiliated with *Betaproteobacteria*, were positively correlated with *Methanosaeta* and *Methanolinea* and coexisted in the HBM and DQN blocks. *Sphingomonas*, *Novosphingobium*, *Brevundimonas*, and *Rhizobium*, affiliated with *Alphaproteobacteria*, were positively correlated with *Methanothermobacter* and coexisted in the DGD, SLZ, and LHA blocks. The existence of diverse microbes with similar functions may increase the biodiversity of the microbiota. Based on the diversity-stability theory, high-diversity systems tend to be robust and resilient (McCann, 2000; Mazancourt et al., 2013).

The dynamic pattern of the ecological relationships between different microbes includes symbiosis, competition, and parasitism (Grossart et al., 2001). Microbes show a trade-off between growth, reproduction, restoration, and resistance under conditions of limited availability of energy sources. Furthermore, microbes compete and cooperate to maintain growth and obtain energy. Our results indicate that abiotic factors, particularly temperature, depth, and the presence of the core archaea, lay the foundation for the microbial network. Furthermore, abundant microbial interactions enrich the microbial network and increase the stability and elasticity of the energy flow in petroleum reservoirs.

3.3. Feasibility and challenge of thermodynamic constraints on microbial community assembly

Our results of null model analysis indicated that the microbiota of the petroleum reservoirs was shaped by deterministic processes. Abiotic factors, particularly temperature and depth, shaped the core archaeal microbiota, which are among the most important participants in the metabolic steps of the methanogenic degradation of petroleum hydrocarbons. Abiotic factors and the core archaeal microbiota then lay the foundation for the microbial food web.

A petroleum reservoir is a chemosynthetically driven ecosystem characterized by a relatively simple carbon source and stable geochemical conditions compared with those in the soil and ocean (Tedersoo et al., 2014; Larsen et al., 2015). The methanogenic degradation of crude oil hydrocarbons shows relatively clear thermodynamic constraints (Dolfing et al., 2008; Dolfing et al., 2009). In our study, the change in the Gibbs free energy, based on thermodynamic reactions, indicated that HMAs preferred high-temperature petroleum reservoirs, whereas AMAs and HAMA preferred low-temperature petroleum reservoirs. This result was consistent with the abundances of the functional archaea determined across our samples using 16S rRNA sequencing (Fig. 5). This result is in agreement with previous findings showing that HMAs are transformed to AMAs under high CO_2 concentrations, which is more thermodynamically favorable (Mayumi et al., 2013). Our results suggest that microbial community assembly is thermodynamically driven.

The elucidation of the intrinsic assembly mechanism is a central goal in ecology. However, complex multifactor, multivariate, and multilevel ecosystems mask this underlying mechanism. The cryosphere of the Earth is a simple ecosystem that includes sea ice, glacial, and subglacial habitats, with a reduced content of organic matter inhabited by diverse organisms. In sea ice and supraglacial habitats, sunlight penetrates the ice. Photoautotrophy, mostly contributed by sea-ice diatoms, serves as the basis for complex food webs, whereas in subglacial habitats, chemoautotrophy is observed (Boetius et al., 2015; Hellweger et al., 2014). The overwhelming majority of microbes in these environments are difficult to culture and model. Therefore, we encountered obstacles in trying to determine the energy flow of these microbes. For these reasons, assessing microbial community assembly based on thermodynamic constraints remains a key challenge in microbial ecology.

4. Conclusion

To date, little is known about the underlying mechanism of microbial community assembly. In this study, the bacterial and archaeal communities in eight Chinese petroleum reservoirs were comprehensively investigated under heterogeneous geochemical conditions to identify the intrinsic mechanism of microbial community assembly. In the petroleum reservoirs, abiotic factors (temperature, depth, TOC, pH, AH, and ASP) significantly influenced the microbiota. Abiotic factors influenced the archaeal communities more than the bacterial communities. The combination of abiotic factors, especially temperature and depth, and the core archaeal genera, including *Archaeoglobus*, *Methanobacterium*, *Methanothermobacter*, unclassified *Methanobacteriaceae*, *Methanomethylovorans*, *Methanoculleus*, *Methanosaeta* and *Methanolinea*, lay the foundation for the bacterial community structures. Null model analysis reflected that deterministic processes shaped the microbial community structures in Chinese petroleum reservoirs. The correlation coefficients between the core archaea relative abundances and temperatures indicated that microbial community assembly in these deep terrestrial ecosystems tended toward a thermodynamically favored state. These findings will lead to new horizons for exploring the assembly mechanisms of various ecological habitats.

5. Materials and methods

5.1. Sampling and analysis of the physico-geochemical characteristics of the water samples

From 2009 to 2010, a total of 50 water samples collected from eight injection wells and 42 production wells of eight water-flooding Chinese oil reservoirs were collected. The eight sampling blocks were XJT (T) and XJQ (Q) in Xinjiang Province, HBM (M) and HBB (B) in Inner

Mongolia Province, DQN (N) in Heilongjiang Province, LHA (A) in Jilin Province, DGD (D) in Tianjin Province and SLZ (Z) in Shandong Province. Physical characteristics of the petroleum reservoirs, such as permeability (PER), porosity (POR), temperature, and depth, were recorded. The distribution of the sampling sites and detailed information on the samples are shown in Fig. 1 and Table S2. All samples were immediately transported to the laboratory, centrifuged at 500 ×*g* to discard the precipitates, and then the upper-phase crude oil and the lower-phase solutions for each sample were separately stored at −80 °C for further analysis. Soon after all 50 water samples were there, the chemical indices of floating crude oil, including sulfur (S), nitrogen (NI) and the contents of four subfractions (wt/wt) (saturated hydrocarbons (SH), aromatic hydrocarbons (AH), nonhydrocarbons (NH), and asphaltene (ASP)) were determined. Meanwhile, the chemical characteristics of the injection water and production water, such as the pH, total organic carbon (TOC), and total salinity degree (TSD), which included anions (Cl^-, NO_3^-, and SO_4^{2-}) and cations (Na^+, K^+, Mg^{2+}, and Ca^{2+}), were also analyzed. All analyses were performed according to the methods of *Tang* et al. (Tang et al., 2012).

5.2. Microbe collection and DNA extraction

For the microbiota composition analysis, microbes from the water samples were collected soon after they arrived at the laboratory by filtering approximately 200–250 ml samples through 0.22-μm hydrophilic membrane filters (Φ47 mm, Millipore, USA). DNA was extracted using the FastDNA® Spin Kit for Soil (MP Biomedicals, Cleveland, USA) according to the manufacturer's instructions and was quantified using a spectrophotometer (Pharmaspec UV-1700, Shimadzu, Kyoto, Japan). The extracted DNA mixture from every sample was stored at −80 °C for further operation.

5.3. Sequencing library construction and pyrosequencing

After DNA mixtures in each of the 50 water samples were obtained, they were processed for the amplicon 454 pyrosequencing. The first step was DNA library construction. For bacterial community analysis, the ~192 bp V3 region of the 16S rRNA gene was amplified with a bacterial universal primer pair 341F/533R (Koike et al., 2007). For archaeal community analysis, nested PCR was performed to amplify the V3-V6 region (approximately 709 bp). The first primer pair was 109F/1386R, followed by 339F/1048R (Jeyanathan et al., 2011). The primers 341F, 533R, and 339F were linked with 454 Life Sciences adaptor sequences, a unique 10-bp error-correcting Golay barcode, and a 'T' linker sequence that was inserted between the barcode and primer, while primer 1048R only harbored the adapter sequence. Three biological replicates were performed for each experiment. All amplicons were visualized using 2% (*w*/*v*) agarose gels (TaKaRa, Japan) and purified using a DNA gel extraction kit (BioTek, China). Purified amplicons of the same sample were mixed in equimolar ratios, followed by sequencing on the 454 Life Sciences Genome Sequencer FLX Titanium platform (Shanghai Majorbio Bio-Pharm Technology Co., Ltd. and TEDA Institute of Biological Sciences and Biotechnology, Nankai University, China). The obtained nucleotide raw data containing the basecalled sequences and corresponding quality scores for all reads were saved in SFF (standard flowgram format) files.

5.4. Pyrosequencing data availability

The SFF files obtained from the 454 sequencer were converted into FASTQ format using Mothur 1.10.2, and then sequences from different samples were discriminated according to the barcodes. The sequences in the distinguished FASTQ files were termed as valid sequences. For bacterial community analysis, valid sequences were optimized for the preferences of both the forward and reverse primers, allowing up to two mismatches, with perfect primer and barcode sequence matching, no ambiguous base calls, a 100-bp minimum sequence length, and more than 30 sequences. For archaeal community analysis, valid sequences were processed using QIIME2–2018.11 (Bolyen et al., 2019) to obtain optimized sequences, which removed ≤200 bp and ≥ 1000 bp sequences, ambiguous bases exceeding 6 bp, a missing qual score or a mean qual score below 25, max homopolymer runs exceeding 6 bp, no mismatches between primers, and uncorrected barcodes. All optimized sequences were compared by using BLASTN with a reference database based on the SILVA database (version 106) and then clustered into operational taxonomic units (OTUs). OTUs were defined according to a farthest neighbor Jukes-Cantor distance of 0.03 and assigned taxonomically using the Ribosomal Database Project (RDP) Naive Bayes classifier. The Shannon-Wiener, Simpson, Chao1, and Good's coverage indices were estimated to determine the diversity of the bacterial and archaeal communities. The sff files were deposited at DDBJ (http://www.ddbj.nig.ac.jp) under the accession numbers listed in Table S2.

5.5. Processing of statistical analyses

Statistical analyses were performed using R software (v.3.4.2, R Project for Statistical Computing). To analyze the heterogeneity of the geochemical conditions, including PER, POR, temperature, depth, TSD, TOC, pH, S, NI, SH, AH, NH, and ASP, in different petroleum reservoirs, principal component analysis (PCA) was performed on a geochemical data matrix using the *pca2d* function in the *pca3d* package of R. The *cor* and *cor.test* functions in the stats package of R were used to calculate and test Spearman's rank correlations between geochemical conditions. A Spearman's correlation coefficient (rho, |ρ|) of ≥0.4 and $P < 0.05$ were considered statistically significant (Barberán et al., 2012).

Based on the frequency of the occurrence of OTUs or genera, the microbes in a single block were divided into three groups: (I) OTUs or genera present in >70% of production water samples in one block were grouped as core OTUs or genera; (II) OTUs or genera present in at least two but <70% of production water samples in one block were grouped as variable OTUs or genera; and (III) OTUs or genera present only in one production water sample were grouped as unique OTUs or genera (Schmitt et al., 2012). Using a similar calculation method, the core, variable, and unique microbes in all blocks were summarized. A Venn diagram based on OTU levels was used to compare the core and variable microbes in the injection and production water samples.

The abiotic and biotic influences on the microbiota were tested using the *envfit* function in the *vegan* package of R based on canonical correlation analysis (CCA) (Werner et al., 2011). $P < 0.05$ based on 999 permutations indicated the significance of geochemical conditions. To more specifically identify the relationships between geochemical conditions and among core and variable microbes in different blocks, the ρ and *P* values of Spearman's rank correlations were calculated. All possible Spearman's rank correlations ($|\rho| \geq 0.4$, $P < 0.05$) were considered valid influencing events, and the topology of the network was described in Cytoscape 3.2.1. The nodes in the reconstructed network represent the geochemical conditions and core-variable genera, whereas the lines correspond to a strong and significant correlation between nodes. Path lines document only the positive and negative correlations, regardless of connectivity (ρ). Node size roughly describes the relative abundance of core microbes.

β-diversity (Bray-Curtis dissimilarity and Jaccard's dissimilarity) represents compositional variations among communities across various spatial scales and provides insights into mechanisms of community assembly (Zhou et al., 2014; Chase, 2010). We calculated the dissimilarity (1-similarity) of the microbiota based on OTU levels using the *vegdist* function in the *vegan* package of R. In the null mode analysis, microbiota assembly via a stochastic process, in which the microbial composition is not regulated by abiotic and biotic factors, was set as the null model. Permutational analysis of multivariate dispersions (PERMDISP) was used to discern whether differences in similarity in the same block were different from the null expectation. The proportions of

deterministic and stochastic processes provided a quantitative estimation of the extent of niche-based deterministic selection in shaping the community composition and structure (Zhou et al., 2014). The analysis of the correlations between the microbiota and geochemical conditions was conducted with a multiple regression model using the *lm* function in the stats package of R (Tedersoo et al., 2014).

5.6. Evaluating the thermodynamics of methanogenic hydrocarbon degradation routes

The degradation of either saturated hydrocarbons ($C_{16}H_{34}$ and $C_{100}H_{202}$) or aromatic hydrocarbons (C_6H_6) are divided into the following two steps.

Step 1: Hydrocarbon oxidation has three types of reactions:

(I) Complete oxidation:

$$4C_xH_y + 8xH_2O \rightarrow 4xCO_2 + (8x + 2y)H_2 \quad (1)$$

(II) Incomplete oxidation to produce acetate:

$$4C_xH_y + (4x-y)H_2O + yCO_2 \rightarrow (2x + y/2)CH_3COOH \quad (2)$$

(III) Incomplete oxidation to produce acetate and H_2:

$$4C_xH_y + 4xH_2O \rightarrow 2xCH_3COOH + 2yH_2 \quad (3)$$

Step 2: Acetate degradation to methane has two types of reactions:

(I) Syntrophic acetate oxidation (acetate oxidation + hydrogenotrophic methanogenesis):

$$(2x + y/2)CH_3COOH + (4x + y)H_2O \rightarrow (4x + y)CO_2 + (8x + 2y)H_2 \quad (4)$$

$$(8x + 2y)H_2 + (2x + y/2)CO_2 \rightarrow (2x + y/2)CH_4 + (4x + y)H_2O \quad (5)$$

(II) Aceticlastic methanogenesis:

$$(2x + y/2)CH_3COOH \rightarrow (2x + y/2)CO_2 + (2x + y/2)CH_4 \quad (6)$$

The Gibbs free energy of each chemical reaction was calculated according to the study by *Dolfing* et al., and temperature corrections for ΔG^0 were performed using the Gibbs-Helmholtz equation: $\Delta G^0_{Tact} = \Delta G^0_{Tref} \cdot \left(\frac{T_{act}}{T_{ref}}\right) + \Delta H^0_{Tref} \cdot \frac{T_{ref} - T_{act}}{T_{ref}}$, with the temperature in Kelvin; T_{ref}= 298.15 K (Dolfing et al., 2008; Dolfing et al., 2009).

CRediT authorship contribution statement

Jie-Yu Zhao: Investigation, Formal analysis, Writing – original draft. **Bing Hu:** Validation, Visualization, Writing – review & editing, Funding acquisition. **Jan Dolfing:** Data curation, Writing – review & editing. **Yan Li:** Conceptualization. **Yue-Qin Tang:** Writing – review & editing. **Yiming Jiang:** Software. **Chang-Qiao Chi:** Resources. **Jianmin Xing:** Writing – review & editing. **Yong Nie:** Project administration, Supervision, Writing – review & editing. **Xiao-Lei Wu:** Supervision, Writing – review & editing, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

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