Supplemental Material

Calcite U-Pb ages constrain petroleum migration pathways in tectonic complex basins

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This supplementary material consists of four parts:

- S1. Tectonic events of the Tarim basin;
- S2. Methods: calcite U-Pb geochronology and fluid inclusion analysis;
- S3. Sample information: Hand specimen, fluid inclusion occurrence, fluorescence spectra and U-Pb ages;
- S4. Source rock maturity and petroleum generation modelling.

S1. Tectonic events of the Tarim basin

Figure S1.1. Compilation of major tectonic events in the Tarim Basin since 500 Ma. Tectonic events are from He et al., (2011), Zhang et al. (2013) and He et al., (2016).

S2. Methods: calcite U-Pb geochronology and fluid inclusion analysis

S2.1 Calcite U-Pb geochronology

Calcite U-Pb analyses were performed at the University of California, Santa Barbara using a Photon Machines Excite 193 laser ablation system coupled to a Nu Instruments Plasma3D multicollector ICP-MS, following the analytical procedures of Kylander-Clark et al. (2020). For each investigated sample, calcite was measured in

80–100 μm sections mounted on glass slides, using an 85 μm spot run at 10 Hz for 15 s following a 20 sec baseline. Unknown analyses were corrected for instrument drift and mass-bias in a 2-step procedure using a combination of analyses from NIST614 glass and calcite standard WC-1 (254 Ma; Roberts et al., 2017) that were measured periodically throughout the analytical session; NIST614 is first used to correct for instrument drift of all isotopic ratios and the mass and detector bias of the $^{207}\text{Pb}/^{206}\text{Pb}$ ratio using Iolite v2.5 (Paton et al., 2011), and a correction for the mass and detector bias of the $^{206}\text{Pb}/^{238}\text{U}$ ratio is corrected such that, using an initial $^{207}\text{Pb}/^{206}\text{Pb}$ ratio of 0.85, WC-1 yields 254 Ma. Uncertainties on individual ratios include 2%, added in quadrature, such that secondary reference materials yield a reasonable MSWD (0.88–1.8 as shown below in this section). Analyses of calcite standards ASH 15D (2.965; Nuriel et al., 2021), Duff Brown Tank (64 Ma; Hill et al., 2016), AUG-B6 (43 Ma; Brigaud et al., 2021) analyzed throughout the analytical session yielded ages that overlap within uncertainty of their accepted values: 2.937 ± 0.098 Ma ($n = 29$; MSWD = 1.05), 66 ± 3 Ma ($n = 10$; MSWD = 1.8), 42.83 ± 0.33 Ma ($n = 42$; MSWD = 0.88), respectively (all unanchored); WC-1 yielded 254.94 ± 0.98 Ma (anchored; $n = 81$; MSWD = 1.5). Given the reproducibility of the secondary reference and the long-term reproducibility of all U-Pb standards, we estimate 2.5% uncertainty of calculated ages; this uncertainty—stated in brackets—is added in quadrature to the analytical uncertainty (stated first). Data points that possess the following characteristics were excluded: (1) data that had uncertainties of 100% or greater; (2) and/or data in which more than half the analysis was within 3s of the baseline (approx. 10% of total data); or (3) data which do not intersect concordia when plotted through a reasonable intercept (<1% of total data). All uncertainties are plotted and quoted at 2σ level.

S2.2 Fluid inclusion analysis

Fluid inclusion petrography and fluorescence spectra measurements were carried out at the Key Laboratory of Deep Oil and Gas in China University of Petroleum (East China), and were performed on a NIKON Ni-U microscope fitted with an ultra-violet (UV) light source. Samples were all prepared as one doubly-polished thin section and one doubly-polished thick section ($\sim 100\mu\text{m}$). Thick sections were used to identify the occurrence of oil inclusions, acquire the fluorescence spectra of primary fluid inclusions and the identify the regions for in-situ U-Pb dating, and thin sections were used to determine the fluorescence spectra of all types of oil inclusions (i.e., primary, secondary oil inclusions and pseudo-secondary if observed). The UV fluorescence spectroscopic analysis of oil inclusions was carried out following the procedure outlined in Ping et al., (2019, 2020), which was measured with a 420 nm barrier epifluorescence filter coupled with a high-pressure mercury lamp with a multichromatic excitation wavelength of 330–380 nm (with peak intensity at 365 nm).

The UV fluorescence spectroscopy measurements were taken in 0.471-nm increments from 420 nm to 800 nm using a 50x objective with an Ocean Optics Maya 2000 pro spectrometer linked to Yuanon software for data acquisition and processing.

S3. Sample information: Hand specimen, fluid inclusion occurrence, fluorescence spectra and U-Pb ages

Calcite samples that were successfully dated with meaningful isochrons are mainly fracture-filling veins (12), with minor portions of pore-filling cement (1) or cement in (tectonic) stylolites (5) (Table S3.1). Fracture-filling veins are all blocky veins with only one generation of growth showing well-developed growth competition textures, except for sample no.6 (JY2 well, 9094.18) which displays obvious crack-seal characteristics (i.e., parallel inclusion bands of wall-rock and oil inclusions arranged parallel to the vein growth fronts), typical of multiple episodes of fracture and sealing (Fig. S3.6). Accordingly, we suspect that the high MSWD (5.6) and relatively large age spread in the T-W isochron of sample no.6 could be explained by mixed ages of multiple crack-seal events in the dated calcite vein, or alternatively explained by variable initial lead. The high MSWD in the T-W isochrons of sample no. 8 (JY7 well, 7108.63m) and no.17 (RP7 well, 6861.89m) might be explained by underestimated analytical uncertainties, mobilization of Pb or U due to open system behaviors or mixed age due to multiple episodes of precipitation. The large age spreads in the T-W isochrons of samples no.10 (YueM5 well, 7267.25m) and no.11 (YueM5 well, 7274.84m) are caused by limited spread in $^{238}\text{U}/^{207}\text{Pb}$ (Table S3.1; Fig. S3.10, S3.11).

Most of the observed oil inclusions are two-phase $\text{L}_{\text{oil}}\text{--V}$ at room temperature (21 °C [69.8 °F]), trapping liquid phase (i.e., colorless-yellow-brown oil) with small vapor phase. One-phase L_{oil} and $\text{S}_{\text{bitumen}}$ inclusions, three-phase inclusions including $\text{L}_{\text{oil}}\text{--L}_w\text{--V}$ and $\text{L}_{\text{oil}}\text{--V--S}_{\text{bitumen}}$ and multi-phase $\text{L}_w\text{--L}_{\text{oil}}\text{--S}_{\text{bitumen}}\text{--V}$ were also observed. Most inclusions display simple ellipsoidal, rectangle or irregular complex shapes of 3-12 μm in diameter. Under UV-epifluorescence, oil inclusions show variable colors, including yellow-green, blue-green and blue-white fluorescence. The shift of fluorescent color from yellow to blue to white indicate an increase of maturity and multiple stages of petroleum charging.

The terms primary and secondary inclusion assemblages are used here to describe the occurrences of oil inclusions. Primary inclusion assemblages are confined in single crystals, and are thought to be coeval with the host calcite minerals. Primary inclusions are trapped along crystal growth bands/cleavages (e.g., oil inclusions assemblages in sample no. 1, 2, 3, 7, 8, 9, 11, 12, 18) or form cloudy cores in single crystals (e.g., oil inclusions assemblages in sample no. 5, 10, 15, 16) or

randomly distributed in single crystals and becomes deficient approaching growth zone boundaries (e.g., oil inclusions in samples no. 17). Secondary inclusions are arranged in trails and are trapped in healed microfractures that crosscut calcite crystals, thus are supposed to be formed later than the crystallization of calcite crystals (Goldstein and Reynolds, 1994; Goldstein, 2001) (e.g., oil inclusions in sample no. 8). Apart from the classical definition of fluid inclusion occurrence and petrographic criteria to identify them, additional types of primary inclusions are also observed in the studied samples. Oil inclusions arranging in bands parallel to the vein walls are also interpreted to be primary, which were trapped during crack-seal events (Fall et al., 2014) (e.g., inclusions in samples no. 2, 6). In addition, we also observed several fluid inclusion assemblages containing large ($\sim 10\text{--}30\text{ }\mu\text{m}$) two-phase liquid-vapor inclusions in microfractures that are perpendicular to the crack-seal layers (e.g., inclusions in samples no. 13). Following Becker et al. (2010) and Fall et al. (2014), who observed similar inclusions in the Piceance Basin, thus we interpret these inclusions as primary or pseudosecondary inclusions that formed along reentrants or deep etches.

Table S3.1. Summary of sample information, associated U-Pb ages and typical Primary oil inclusion fluorescence. Bracketed numbers in U-Pb age column are quoted uncertainties with systematic uncertainty propagation.

Well	Sample Number	Depth (m)	Dated fabric	U-Pb age (MSWD)	Primary oil inclusion Fluorescence
Ha15-33	no.1	6617	fracture-filling vein	272.2 $\pm$ 2.1 [7.2] (0.65)	559.2nm
Ha6-1	no.2	6669	fracture-filling vein	444.4 $\pm$ 1.9 [11.3] (1.2)	543.47nm
Ha702	no.3	6654.2	pore-filling cement	434.6 $\pm$ 2.9 [11.3] (0.92)	541.67nm
JY103	no.4	7241.5	fracture-filling vein	293.9 $\pm$ 2.8 [7.9] (0.96)	516.37nm
JY103	no.5	7241.6	fracture-filling vein	440 $\pm$ 17 [20.3] (1.5)	543.47nm
JY2	no.6	7094.18	fracture-filling vein	371 $\pm$ 39 [40.1] (5.6)	539.86nm
JY7	no.7	7108.63	fracture-filling vein	286 $\pm$ 16 [17.5] (1.5)	511.39nm
JY7	no.8	7108.63	fracture-filling vein	262.5 $\pm$ 6.9 [9.6] (4.2)	515.02nm
YueM1	no.9	7266.17	fracture-filling vein	475 $\pm$ 19 [22.4] (0.63)	516.37nm
YueM5	no.10	7267.25	fracture-filling vein	416 $\pm$ 77 [77.7] (1.9)	513.21nm
YueM5	no.11	7274.84	fracture-filling vein	379 $\pm$ 79 [79.6] (1.8)	511.39nm
YueM6	no.12	7306.48	fracture-filling vein	443 $\pm$ 27 [29.2] (1.4)	515.02nm
YueM6	no.13	7306.5	fracture-filling vein	442.0 $\pm$ 8.7 [14.1] (0.86)	518.18nm
RP7	no.14	6862.75	cement in tectonic stylolite	435.5 $\pm$ 2.6 [11.3] (1.8)	548.43nm
RP7	no.15	6868.81	cement in tectonic stylolite	439.0 $\pm$ 3.1 [11.5] (0.97)	546.62nm

RP7	no.16	6858.58	cement in tectonic stylolite	433.4±4.0 [11.6] (1.8)	541.67nm
RP7	no.17	6861.89	cement in stylolite	436.7±3.4 [11.5] (1.4)	545.27nm
RP7	no.17	6861.89	cement in stylolite	288.4±8.5 [11.2] (3.9)	513.21nm
JY204	no.18	7150.4	cement in stylolite	454±37 [38.7] (0.45)	539.86nm

Below are detailed sample information, including 1-inch round thick sections used for in-situ U-Pb dating, primary oil inclusion occurrence, typical fluorescence spectra, and representative Tera-Wasserburg concordia plots for dated calcite samples.

Calcite fracture-filling thin vein in sample No.1 collected from Ha15-33 well (6617m) were chosen for in-situ U-Pb dating (Fig. S3.1). Primary yellow-green oil inclusion assemblages were mostly trapped along the growth bands in single calcite crystals in the vein (as outlined by red dashed lines in Fig. S3.1), with representative fluorescence spectra ($\lambda_{\max}$) of 559.2nm. This vein precipitated in 272.2 ± 2.2 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.1.

Figure S3.1. Sample No.1 collected from Ha15-33 well (6617m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling thin vein in sample No.2 collected from Ha6-1 well (6669m) were chosen for in-situ U-Pb dating (Fig. S3.2). Primary yellow-green oil inclusion assemblages were observe to (1) arrange along growth bands in single crystals and (2) arrange in bands parallel to the vein walls indicating trapping during repeated crack-seal events (as outlined by red dashed lines in Fig. S3.2), with representative fluorescence spectra ($\lambda_{\max}$) of 543.47nm. This vein precipitated in 444.4 ± 1.9 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.2.

Figure S3.2. Sample No.2 collected from Ha6-1 well (6669m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite void-filling cement in sample No.3 collected from Ha702 well (6654.2m) were chosen for in-situ U-Pb dating (Fig. S3.3). Primary yellow-green oil inclusion assemblages were mostly trapped along the growth bands in single calcite crystals in the cement (as outlined by red dashed lines in Fig. S3.3), with representative fluorescence spectra (λ_{max}) of 541.67nm. This cement precipitated in 434.4 ± 2.9 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.3.

Figure S3.3. Sample No.3 collected from Ha702 well (6654.2m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling thick vein in sample No.4 collected from JY103 well (7241.5m) were chosen for in-situ U-Pb dating (Fig. S3.4). Primary blue-green oil inclusions were trapped in single calcite crystals the vein bounded by growth zone boundaries (as outlined by red dashed lines in Fig. S3.4), with representative fluorescence spectra (λ_{max}) of 516.37nm. This vein precipitated in 293.9 ± 2.8 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.4.

Figure S3.4. Sample No.4 collected from JY103 well (7241.5m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling thin vein in sample No.5 collected from JY103 well

(7241.6m) were chosen for in-situ U-Pb dating (Fig. S3.5). Primary yellow-green oil inclusions clustered in cloudy cores in single crystals and became deficient approaching growth zone boundaries (as outlined by red dashed circle in Fig. S3.5), with representative fluorescence spectra ($\lambda_{\max}$) of 543.47nm. This vein precipitated in 440 ± 17 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.5.

Figure S3.5. Sample No.5 collected from JY103 well (7241.6m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling thin vein in sample No.6 collected from JY2 well (7094.18m) were chosen for in-situ U-Pb dating (Fig. S3.6). Primary yellow-green oil inclusion assemblages trapped during repeated crack-seal events arrange in bands parallel to the vein walls (as outlined by red dashed lines in Fig. S3.6), with representative fluorescence spectra ($\lambda_{\max}$) of 539.86nm. This vein precipitated in 371 ± 39 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.6.

Figure S3.6. Sample No.6 collected from JY2 well (7094.18m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling thin vein in sample No.7 collected from JY7 well (7108.63m) were chosen for in-situ U-Pb dating (Fig. S3.7). Primary blue-green oil inclusion assemblages were mostly trapped along the growth bands in single calcite crystals in the vein (as outlined by red dashed lines in Fig. S3.7), with representative fluorescence spectra ($\lambda_{\max}$) of 511.39nm. This vein precipitated in 286 ± 16 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.7.

Figure S3.7. Sample No.7 collected from JY7 well (7108.63m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling thin vein in sample No.8 collected from JY7 well (7108.63m) were chosen for in-situ U-Pb dating (Fig. S3.8). Primary blue-green oil inclusion assemblages were mostly trapped along the growth bands/cleavages in single calcite crystals in the vein (as outlined by red dashed lines in Fig. S3.8), with representative fluorescence spectra ($\lambda_{\max}$) of 515.02nm. Secondary blue-white oil inclusion assemblages were also observed, arranging in trails in healed microfractures that crosscut calcite crystals, with representative fluorescence spectra ($\lambda_{\max}$) of 477.33nm. This vein precipitated in 286 ± 16 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.8.

Figure S3.8. Sample No.8 collected from JY7 well (7108.63m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling vein in sample No.9 collected from YueM1 well (7266.17m) were chosen for in-situ U-Pb dating (Fig. S3.9). Primary blue-green oil inclusion assemblages were mostly trapped along the thick growth bands in single calcite crystals in the vein (as outlined by red dashed lines in Fig. S3.9), with representative fluorescence spectra (λ_{max}) of 516.37nm. This vein precipitated in 475 ± 19 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.9.

Figure S3.9. Sample No.9 collected from YueM1 well (7266.17m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling vein in sample No.10 collected from YueM5 well (7267.25m) were chosen for in-situ U-Pb dating (Fig. S3.10). Primary blue-green oil inclusions randomly distributed in cloudy cores in single crystals and terminated against growth zone boundaries (as outlined by red dashed lines in Fig. S3.10), with representative fluorescence spectra (λ_{max}) of 513.21nm. This vein precipitated in $416 \pm 77\text{Ma}$, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.10.

Figure S3.10. Sample No.10 collected from YueM5 well (7267.25m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling vein in sample No.11 collected from YueM5 well (7274.84m) were chosen for in-situ U-Pb dating (Fig. S3.11). Primary blue-green oil inclusion assemblages were mostly trapped along the thick growth bands in single calcite crystals in the vein (as outlined by red dashed lines in Fig. S3.11), with representative fluorescence spectra (λ_{max}) of 511.39nm. This vein precipitated in 379 ± 79 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.11.

Figure S3.11. Sample No.11 collected from YueM5 well (7274.84m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling thin vein in sample No.12 collected from YueM6 well (7306.48m) were chosen for in-situ U-Pb dating (Fig. S3.12). Primary blue-green oil inclusion assemblages were mostly trapped along the growth bands in single calcite crystals in the vein (as outlined by red dashed lines in Fig. S3.12), with representative fluorescence spectra ($\lambda_{\max}$) of 515.02nm. This vein precipitated in 443 ± 27 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.12.

Figure S3.12. Sample No.12 collected from YueM6 well (7306.48m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite fracture-filling thin vein in sample No.13 collected from YueM6 well (7306.5m) were chosen for in-situ U-Pb dating (Fig. S3.13). Primary blue-green oil inclusion assemblages containing large (~ 10 – $30\ \mu\text{m}$) two-phase liquid-vapor inclusions are trapped in trails perpendicular to the crack-seal layers (as outlined by red dashed lines in Fig. S3.13), with representative fluorescence spectra ($\lambda_{\max}$) of 518.18nm. This vein precipitated in 442 ± 8.7 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.13.

Figure S3.13. Sample No.13 collected from YueM6 well (7306.5m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite cement in tectonic stylolite in sample No.14 collected from RP7 well (6862.75m) were chosen for in-situ U-Pb dating (Fig. S3.14). Primary yellow-green oil inclusions randomly distributed in single crystals (as outlined by red dashed lines in Fig. S3.14), with representative fluorescence spectra (λ_{max}) of 548.43nm. This cement precipitated in 435.5 ± 2.6 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.14.

Figure S3.14. Sample No.14 collected from RP7 well (6862.75m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite cement in tectonic stylolite in sample No.15 collected from RP7 well (6868.81m) were chosen for in-situ U-Pb dating (Fig. S3.15). Primary yellow-green oil inclusions randomly distributed in cloudy cores in single crystals and terminated against growth zone boundaries (as outlined by red dashed lines in Fig. S3.15), with representative fluorescence spectra (λ_{max}) of 546.62nm. This cement precipitated in 439 ± 3.1 Ma, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.15.

Figure S3.15. Sample No.15 collected from RP7 well (6868.81m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite cement in tectonic stylolite in sample No.16 collected from RP7 well (6868.81m) were chosen for in-situ U-Pb dating (Fig. S3.16). Primary yellow-green oil inclusions randomly distributed in cloudy cores in single crystals and terminated against growth zone boundaries (as outlined by red dashed lines in Fig. S3.16), with representative fluorescence spectra (λ_{max}) of 541.67nm. This cement precipitated in $433.4 \pm 4\text{Ma}$, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.16.

Figure S3.16. Sample No.16 collected from RP7 well (6858.58m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite void-filling cement along stylolite in sample No.17 collected from RP7 well (6861.89m) were chosen for in-situ U-Pb dating (Fig. S3.17). Two regressions can be plotted in the Tera-Wasserburg concordia plot through all U-Pb dating data points, with an older age of 436.7 ± 3.4 Ma and a younger age of 288.4 ± 8.5 Ma determined (Fig. S3.17). Under microscope with transmitted light and UV epi-fluorescence light, we cannot readily distinguish the two fabrics petrographically. However, we interpret this two ages represent two discrete events of fluid flow and cement precipitation rather than ‘apparent ages’ caused by mobility of U or Pb by recrystallization, based on: (1) relatively low MSWDs of the two isochrons, and distinctly separated datapoints in the two regressions, as compared to typical diagenetic altered partially reset U-Pb isochrons with MSWD 10-100 times larger than produced by reasonable initial heterogeneity (Rasbury and Cole, 2009); (2) uniform initial $^{207}\text{Pb}/^{206}\text{Pb}$ compositions (~ 0.8) between the two isochrons; (3) other samples also revealed similar ages in ~ 450 - 400 Ma and in ~ 290 - 250 Ma, possibly pointing to two extensive tectonic movement and fluid flow events; and (4) no clear petrographic evidence (much larger or smaller crystals than others) showing signs of recrystallization. Two kinds of oil inclusion assemblages were observed: (1) A primary yellow-green oil inclusion assemblage randomly distributed in single crystals and terminated against growth zone boundaries (as outlined by red dashed lines in Fig. S3.17), with representative fluorescence spectra (λ_{max}) of 545.27 nm; (2) and a putative primary blue-green oil inclusion assemblage randomly distributed in single crystal (as also outlined by red dashed lines in Fig. S3.17), with representative

fluorescence spectra (λ_{max}) of 513.21nm. As the two phases of cements cannot be distinguished, we thus assume the lower matured primary yellow-green oil inclusion assemblage were trapped during the precipitation of the ‘older’ cement ($436.7 \pm 3.4\text{Ma}$), and the higher matured putative primary blue-green oil inclusion assemblage were trapped during the precipitation of the ‘younger’ cement ($288.4 \pm 8.5\text{Ma}$). Nevertheless, considering the MSWD (3.9) of the shallower regression ($288.4 \pm 8.5\text{Ma}$), this younger age should be viewed with caution.

Figure S3.17. Sample No.17 collected from RP7 well (6861.89m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

Calcite void-filling cement along stylolite in sample No.18 collected from JY204 well (7150.4m) were chosen for in-situ U-Pb dating (Fig. S3.18). Primary yellow-green oil inclusion assemblages were mostly trapped along the growth bands in single calcite crystals in the cement (as outlined by red dashed lines in Fig. S3.18), with representative fluorescence spectra (λ_{max}) of 539.86nm. This cement precipitated in $454 \pm 37\text{Ma}$, as revealed in the Tera-Wasserburg concordia plot in Fig. S3.18.

Figure S3.18. Sample No.18 collected from JY204 well (7150.4m). MSWD=mean square weighted deviation. All uncertainties in the Tera-Wasserburg diagram are plotted and quoted at 2σ level.

S4. Source rock maturity and petroleum generation modelling

2D Source rock maturity and petroleum generation modeling of the Halahatang oilfield was conducted using the Petromod software. The modelling was conducted on the N-S trending cross section in Figure 1C.

The input parameters include stratigraphic layers, depositional ages, fault properties, facies (including lithology, petroleum system elements and source rock properties) and boundary conditions (including erosion events and associated erosion thickness, paleo water depth, sediment water interface temperature and heat flow).

Stratigraphic layers and lithologies were taken from the well completion reports provided by PetroChina Tarim Oilfield Company. Published thermal conductivity data for different lithology types (Li et al., 2019) were integrated into the model and default parameters in the petromod software were used for the initial porosity, matrix density and heat capacity. Petroleum system elements include a lower Cambrian source rock interval (the Yuertusi Formation, abbreviated as C_1Y), lower to middle Ordovician reservoir intervals (the Yingshan and Yijianfang Formations, abbreviated as O_2Yj and $O_{1-2}Y$, respectively) and upper Ordovician caprock intervals (the Tumuxiuke, Lianglitage and Sangtamu Formations, abbreviated as O_3T , O_3L and O_3S , respectively). As the lower Cambrian source rock was not drilled in the Halahatang oilfield due to its ultra-deep burial depth (~ 9000 - 10000 m), we used the source rock properties from the Luntan 1 well, one of the two wells penetrating the source rock interval in the Tabei uplift, which is located upper north in the Tabei uplift (average

TOC of 9.5%). The petroleum generation kinetics refers to models proposed by Dieckmann et al. (2000).

Erosion events and the according eroded thickness in the Tabei uplift were cited from Liu et al. (2015), who constrained erosion thickness by geophysical methods (e.g., via seismic reflection data and well logs). Heat flow change through time in the Tabei uplift was estimated based on the reference values suggested by Li et al., (2010). Paleo water depth was inferred from the sedimentary facies of stratigraphic formations determined by Liu et al. (2015). Sediment water interface temperature was assigned using the Automatic SWIT Tool in the Petromod 2D software by setting the hemisphere, continental location and latitude of the studied area. Considering the spatial variations of boundary conditions (i.e., erosion, heat flow and paleo water depth and sediment water interface temperature), all boundary conditions were generated using the trend maps by defining the variation trends at each grid locations.

Figure S4.1. Source rock maturity modeling results for five periods in 0 Ma (present day), 199.6 Ma (Indosinian orogeny), 251 Ma (late Hercynian orogeny), 359.2 Ma (early Hercynian orogeny), 415 Ma (late Caledonian orogeny). Note the maturity disparities between the Northern and the Southern areas.

Figure S4.2. Petroleum generation modelling results for three pseudo-wells located in the Northern, Central and Southern areas of the Halahatang oilfield.

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