

Modeling petroleum expulsion in sedimentary basins: The importance of igneous intrusion timing and basement composition

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ABSTRACT

The concept of a *critical moment* in a petroleum system (the time of highest probability of entrapment and preservation of oil and gas) has underlain petroleum exploration for over 25 years. However, one area where understanding the critical moment is challenging is the Faroe-Shetland Basin (FSB; offshore UK). Isotopic dating of oils suggests that petroleum generation began between ca. 68 and 90 Ma; however, most basin models invoke an earlier generation beginning in the mid-Cretaceous at ca. 100 Ma, predating deposition of Paleocene and Eocene reservoirs. This time discrepancy has previously been explained by remigration from intermediary accumulations (“motel” hypothesis) and/or overpressure retardation of kerogen maturation. The FSB is characterized by a thick Cretaceous stratigraphic package (up to 5 km) that includes a large net thickness (up to 2 km) of Paleogene igneous material. In our model, separating sedimentary and igneous material and adding the igneous material at the correct time between ca. 58 and 55 Ma shallows the modeled burial depth of the Upper Jurassic source rocks during the Cretaceous sufficiently to delay maturation by 17 m.y. in comparison to results of previous studies. Additionally, previous studies have invoked crustal radiogenic heat production (RHP) based on the Phanerozoic crust averaging $\sim 2.8 \mu\text{W}/\text{m}^3$ in the North Sea (300 km to the east). However, the FSB basement is composed of significantly older, colder Neoproterozoic orthogneisses (ca. 2.7–2.9 Ga), reducing RHP by up to 50% to $\sim 1.6 \mu\text{W}/\text{m}^3$ ($\sigma = 0.74$). For the first time, our model unifies geological, geochronological, and geochemical observations, delaying the onset of petroleum expulsion by up to 40 m.y. in comparison to previous models.

INTRODUCTION

Within many sedimentary basins affected by volcanic activity, the modeled *critical moment* (depicting the time after petroleum generation, trap formation, and fluid migration with the highest probability of entrapment and preservation of most petroleum) often disagrees with the observations from actual discoveries (e.g., Bohai Bay Basin, northeastern China) (Hao et al., 2007). One such basin is the Faroe-Shetland Basin (FSB), located within the West of Shetland region of the UK continental shelf (Fig. 1).

The FSB is an area of active petroleum exploration, with discovered resources estimated at 1.6 billion barrels of oil equivalent (Oil and Gas Authority, 2018), including the Schiehallion and Rosebank fields. Oil generation from the main source rock, the Upper Jurassic Kimmeridge Clay Formation (KCF), has previously been thought to have started by the mid-Cretaceous based on previous models, due to rapid Cretaceous basin subsidence (Holmes et al., 1999). But this timing significantly predates the deposition of Paleocene and lower Eocene reservoirs and seals in the area, and the development of

structural traps during Miocene inversion along faults at ca. 16 Ma (Tuitt et al., 2010), resulting in a discrepancy between the apparent timing of petroleum generation and trap formation. This discrepancy has previously been explained by invoking either overpressure delaying the critical moment of petroleum generation (Carr and Scotchman, 2003) and/or transitory hypothesized reservoirs (“motels”; Lamers and Carmichael, 1999) operating between the source rock and reservoir that temporarily host migrating petroleum before more-recent remigration into Paleocene reservoirs.

Importantly, large areas of Cretaceous and lower Paleocene sediments across the FSB are intruded by a subsurface sill complex emplaced between 58 and 55 Ma (Schofield et al., 2017). Although previous work has investigated the direct heating effects of intrusions on source rocks within basins (Aarnes et al., 2015; Peace et al., 2017), few have quantitatively considered the additional effects that intruding a net thickness of up to 2 km of igneous material into the overburden above a source rock has on petroleum generation.

Here we demonstrate, using one-dimensional (1-D) and three-dimensional (3-D) basin modeling, that properly estimating the thickness of igneous intrusions within the overburden atop the KCF, and emplacing this at the correct time at ca. 58–55 Ma, results in a later onset of oil generation than previously determined. Crucially, when used in conjunction with a lithospheric thermal model that incorporates the “old and cold” Neoproterozoic basement typical of the FSB, our model delays the critical moment of petroleum generation locally until

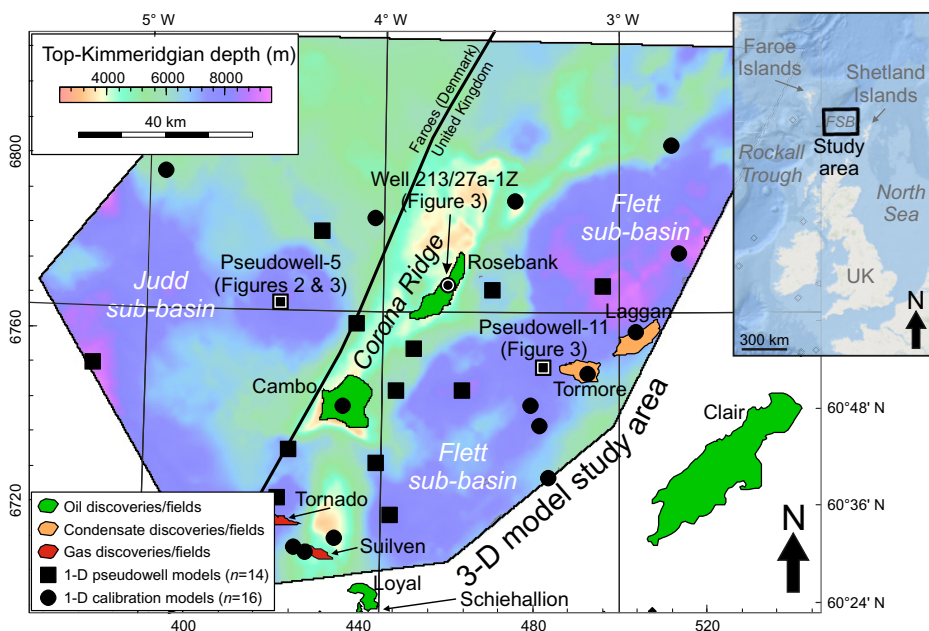


Figure 1. Top-Kimmeridgian source-rock depth map for the Faroe-Shetland Basin (FSB; offshore UK) derived from seismic interpretation, and including the Judd and Flett sub-basins and showing the location of one-dimensional (1-D) models. Coordinate system: ED50, UTM 30N. 3-D—three-dimensional.

after the Paleogene reservoir and seal strata are deposited, removing the need to rely completely on complex remigration modeling such as the “motel” and “whoopie cushion” models of Lamers and Carmichael (1999) and Iliffe et al. (1999), respectively.

PETROLEUM SYSTEMS WITHIN THE FAROE-SHETLAND BASIN

Organic geochemical interpretations suggest that the primary source rock of most oils within the FSB is the locally oil-prone, lacustrine–fluvio-deltaic–marginal marine shales of the Upper Jurassic to Lower Cretaceous KCF (Scotchman et al., 2018). Isotopic dating of oils and fluid inclusions indicates a range of implied petroleum generation ages, from 68 ± 13 Ma based on Re-Os isotopes (Finlay et al., 2011), to 69–93 Ma from U-Pb dating of calcite mineralization (Holdsworth et al., 2019), to ca. 83 Ma from Ar-Ar dating of feldspars surrounding oil-filled inclusions (Mark et al., 2005).

TIME DISCREPANCY IN PETROLEUM SYSTEM MODELING

The timing conundrum between the onset of petroleum generation, charge timing, and reservoir and trap availability has been previously explained by Iliffe et al. (1999) and Lamers and Carmichael (1999), who inferred the storage of petroleum in deep Cretaceous reservoirs prior to geologically recent re-migration into Paleogene reservoirs. However, the presence of Cretaceous sandstones with porosity and permeability remains unproven (Scotchman et al., 2006), and there is little evidence of widespread oil staining

or fluid inclusions within Cretaceous strata in the FSB (Doré et al., 1997).

Carr and Scotchman (2003) provided an alternative mechanism for delay of the onset of oil generation until the Cenozoic by invoking the overpressure of the source rock to retard kerogen (the organic matter within a source rock with generates bitumen during petroleum generation) transformation. However, the quantitative impact of overpressure on kerogen maturation remains a subject of debate (Huang, 1996; Landais et al., 1994). In addition, the magnitude of overpressure varies markedly across the FSB (Iliffe et al., 1999), calling into question the viability of employing this model regionally. Schofield et al. (2017) and Mark et al. (2018) both suggested that removal of igneous intrusions and restoration of the original basin sedimentary thickness may lead to later burial and onset of oil generation within the FSB than previously assumed, but this was not quantified.

QUANTIFYING PALEOGENE IGNEOUS MATERIAL AND PARAMETERS FOR BASIN MODELING

To resolve the controversy (or discrepancy) regarding the timing of petroleum generation, we constructed a 3-D basin model using ZetaWare, Inc. Trinity T3 software (<https://www.zetaware.com/products/t3/index.html>), and thermally calibrated it to 30 1-D models calibrated to present-day temperature and vitrinite reflectance data using a transient, lithospheric model utilizing the crustal structure reported by Ripington et al. (2015). Detailed modeling inputs,

outputs, and rationale are provided in the supporting material in the GSA Data Repository¹.

INCLUSION OF IGNEOUS MATERIAL IN CRETACEOUS SEQUENCES IN THE FSB

Mark et al. (2018) showed that the Cretaceous thickness within the FSB, previously assumed to be of sedimentary origin, is commonly a combined thickness of both Cretaceous sedimentary material and a substantial thickness of Paleogene-aged sills, producing an “overthickening” of the Cretaceous sequences post-deposition. Crucially, this forms a significant proportion of the overburden above the Jurassic source rocks (Schofield et al., 2017).

Imaged and unimaged igneous intrusions can locally have a cumulative thickness totaling 1–2 km (out of a typical 3–5-km-thick Cretaceous section), which needs to be removed to restore the Cretaceous section to its original depositional thickness. The major implication of removing igneous material is that Jurassic source rocks were significantly shallower than previously considered, and thus colder, until ca. 58–55 Ma.

Because ~91% of measured intrusions in FSB wells are <40 m in thickness and typically basaltic in nature (Mark et al., 2018), our model suggests geologically rapid cooling of intrusions (on the order of 10^2 to 10^4 yr) due to the large contact area with surrounding country rock sediments and the relatively rapid heat conduction associated with thin intrusions (Peace et al., 2017).

The Cretaceous sediments within the FSB are primarily shales and other fine-grained rocks, which typically have low thermal conductivities, averaging ~0.8–1.5 W/(m·K) globally (Sharma, 2002). This results in a relatively high geothermal gradient (>35 °C/km), with a shallow depth (<2.5–3.0 km) to the oil-generation window (90–140 °C) in the FSB. In contrast, crystalline igneous material is an efficient conductor of heat, with the thermal conductivities of dolerite ranging from ~2.1 to 2.5 W/(m·K) (Hartlieb et al., 2016).

We estimate that including crystalline igneous material in our model may result in up to a 36% increase in the net thermal conductivity of the Cretaceous overburden above the KCF (based on 100% sediment versus 50% sediment and 50% igneous material), invoking a reduction of up to ~8% in the geothermal gradient of the Cretaceous package wherever intrusions are thickest, and reducing the present-day temperature of the underlying KCF. Where the top KCF is overlain by up to 7 km of overburden, this may amount to a reduction of up to 20 °C at

¹GSA Data Repository item 2019328, supplementary data (geochemical summary, rationale and data tables), is available online at <http://www.geosociety.org/datarepository/2019/>, or on request from editing@geosociety.org.

the top KCF level at the present day, compared to sedimentary overburden alone in our model.

The model indicates that in the center of the Judd sub-basin, KCF oil generation begins as early as ca. 90 Ma when modeling the total Cretaceous thickness, because of the implied thick, poorly thermally conductive Cretaceous (i.e., mud-rich) overburden (Fig. 2B). However, with emplacement of the 1190 m thickness of Paleogene intrusions predicted in this location by Mark et al. (2018) at the correct time (58–55 Ma), the thinner overburden during the Upper Cretaceous above the KCF would reduce the source rock paleotemperature, with the predicted onset of petroleum generation in the late Campanian (73 Ma), ~17 m.y. closer to the present day than in previous models (Fig. 2B).

Interestingly, the relatively high thermal conductivity of crystalline igneous rocks in comparison to mud-rich sediments within the overburden atop the KCF is calculated to have a significant influence on maturation history, resulting in up to a 7% decrease in the geothermal gradient at present day where intrusions are thickest.

However, even after including 1190 m of intrusive material, the model suggests that oil generation in the center of most sub-basins in the FSB would still have begun within the Cretaceous. This implies that additional processes must be considered to allow oil expulsion to have begun in the Cenozoic.

INCLUSION OF NEOARCHEAN BASEMENT

Lithospheric composition and structure act as primary controls on the thermal regime in sedimentary basins, with up to 50% of surface heat flow originating from radiogenic heat production (RHP) from the upper crystalline crust and basin infill (Vilà et al., 2010). The RHP from “typical” Phanerozoic continental crust (including the North Sea) ranges from 2.5 to 3.2 $\mu\text{W}/\text{m}^3$ (Pollack and Chapman, 1977), with default values of upper-crust RHP in most basin modeling software (e.g., Genesis [https://www.zetaware.com/products/genesis/index.html], PetroMod [https://www.software.slb.com/products/petro-mod]) set at ~2.8–3.2 $\mu\text{W}/\text{m}^3$.

The basement underlying the FSB is composed Neoproterozoic (ca. 2.7–2.8 Ga) orthogneisses (Holdsworth et al., 2018) that typically contain low concentrations of heat-producing radionuclides ^{40}K , ^{232}Th , ^{235}U , and ^{238}U (Pollack and Chapman, 1977), which, together with the prolonged time for radiogenic decay, are expected to result in cold (reduced RHP) basement at the time of petroleum generation.

To test this, we calculated RHP using K, Th, and U concentrations following the method of Turcotte and Schubert (2014) from three basement samples from wells in the study area: 204/10-1 (Amerada Hess Corporation, 2002), 205/16-1 (BP, 1986) and 214/9-1 (Total, 2000). The result is a mean RHP of 1.6 $\mu\text{W}/\text{m}^3$ ($\sigma = 0.74$), a reduction of up to 50% in comparison to a “typical” North Sea value of 3.2 $\mu\text{W}/\text{m}^3$.

Without incorporating igneous intrusions, this “cold” basement results in a mean present-day surface heat flow of $51.6 \pm 2.5 \text{ mW}/\text{m}^2$ and a geothermal gradient of $30.7 \pm 2.8 \text{ }^\circ\text{C}/\text{km}$ across the FSB, a decrease of ~10% in comparison to a “typical” North Sea RHP model. This “cold”

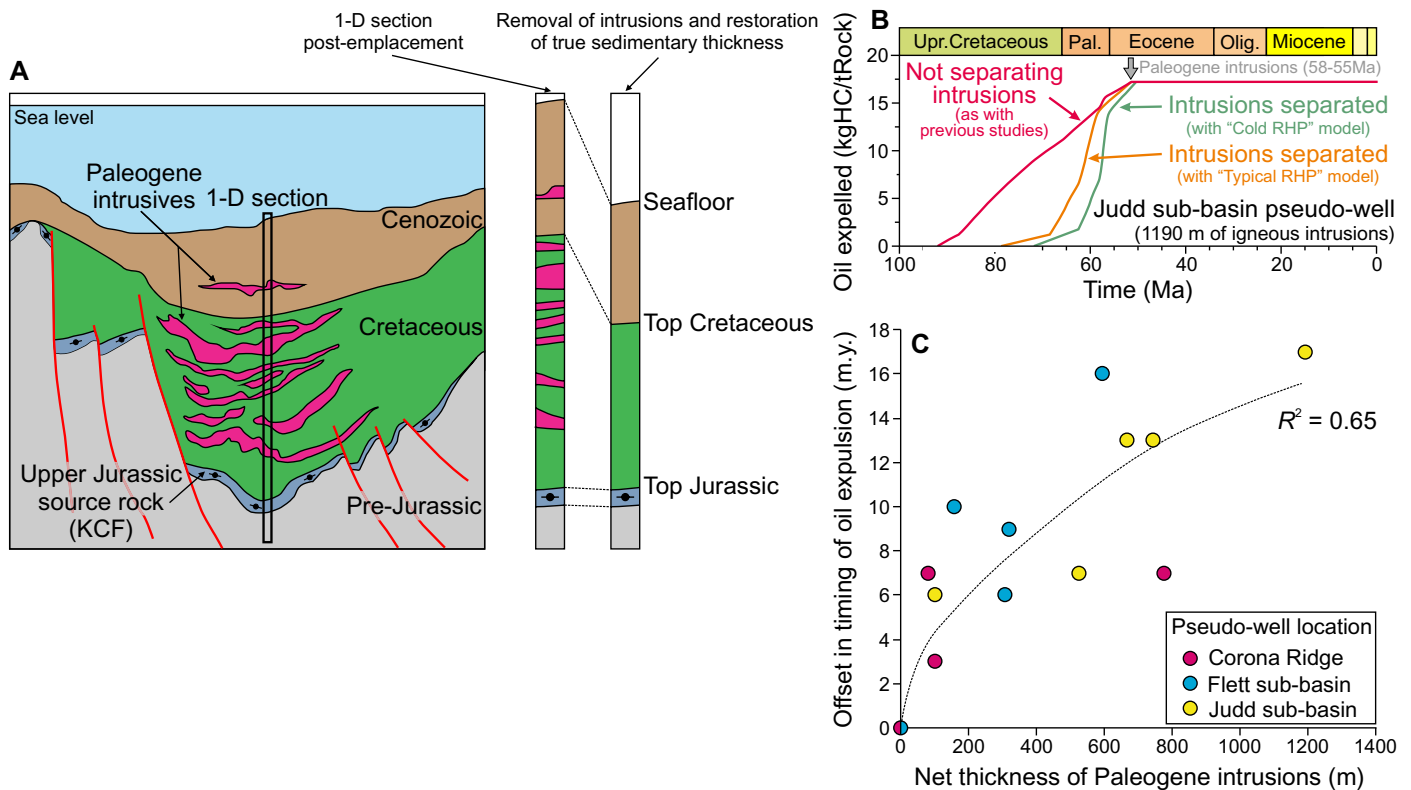


Figure 2. (A) Schematic concept, modified from Mark et al. (2018), of “overthickening” of a sedimentary section in the Faroe-Shetland Basin (FSB; offshore UK) by igneous intrusions, and the need to add igneous intrusions into the overburden atop the source rocks at the correct time (58–55 Ma). KCF—Kimmeridge Clay Formation; 1-D—one-dimensional. (B) Modeled oil expulsion (kilograms of hydrocarbon per ton of rock) history from Kimmeridgian source rock in a 1-D pseudo-well model (constructed from seismic data in locations of specific interest to investigate the burial, thermal, and maturity history; e.g., source rock kitchens, un-drilled prospects) from the center of the Judd sub-basin (based on stratigraphic tops from seismic data), highlighting the impact of “overthickening” assuming a net thickness of 1190 m of igneous intrusions within the Cretaceous and Paleogene overburden, with both “typical radiogenic heat production (RHP)” (2.8 $\mu\text{W}/\text{m}^3$) and “cold RHP” (1.6 $\mu\text{W}/\text{m}^3$) crust of the North Sea and Neoproterozoic orthogneiss basement in the FSB, respectively. The variable heat flow history used broadly matches that of Iliffe et al. (1999), including three phases of rifting (early Cretaceous [145–130 Ma], Albian [110–100 Ma], and Campanian [85–80 Ma]) and the heat “pulse” associated with Paleogene volcanism (58–55 Ma). Upr.—Upper; Pal.—Paleocene; Olig.—Oligocene. (C) Relationship between net igneous intrusion thickness and time difference of onset of oil expulsion for 14 1-D pseudowell models located in Figure 1.

basement model suggests that the onset of oil expulsion would have occurred later than previously predicted, by as much as 30 m.y. in the center of the Judd sub-basin and as much as 22 m.y. in the center of the Flett sub-basin (Fig. 3).

DISCUSSION: MOTEL MODELS, OVERPRESSURE, BASEMENT COMPOSITION, OR IGNEOUS OVERTHICKENING?

We have demonstrated that considering an appropriate basement composition, in conjunction with both the post-deposition thickening and increase in thermal conductivity of the Cretaceous overburden by Paleogene igneous intrusions, the onset of KCF oil expulsion may have begun as much as 40 m.y. later than previously modeled (Fig. 2B), within the isotopic age range of oils (Fig. 3).

However, as demonstrated by Mark et al. (2018), the presence and thickness of Paleogene intrusions are highly variable across the FSB,

from as much as 2 km in the Nuevo sub-basin to 200 m locally in the Flett sub-basin, ~30 km away. We therefore argue that no one unifying mechanism across the basin can solely explain the time discrepancy between basin models and the actual timing of petroleum charge. Rather, the mechanisms outlined in this paper, combined with previous models (e.g., overpressure retardation and “motel” models) or some hitherto unrecognized factors, might all operate across the FSB to some degree. Our model cannot account for the very recent charge (since 20 Ma) seen in many fields within the FSB, based on the modeled biodegradation rate of oils and reservoir temperature histories. On this basis, re-migration of oil from basin sands or long-lived open fracture systems in the basement (Holdsworth et al., 2019) could provide the source of oil required for recent replenishment of oil fields and discoveries in the basin margins. Igneous intrusions may act as migration barriers within the heavily intruded sections of the basin, providing a complex migra-

tion route to accumulations on the basin margins (Rateau et al., 2013).

What is clear, however, is the importance of considering all rocks within and beneath a basin, both sedimentary and crystalline. The properties of the non-sedimentary rocks and their true age and composition must be accurately accounted for if the basin model is to reflect reality.

CONCLUSIONS

We have shown the key elements needed to predict the critical moment of petroleum generation in basins that contain substantial igneous intrusion and/or variations in basement composition. The three main factors that should be considered when undertaking basin modeling in such circumstances are

1. The addition of intrusive igneous material at the correct time in order to correctly model the subsidence history of the petroleum

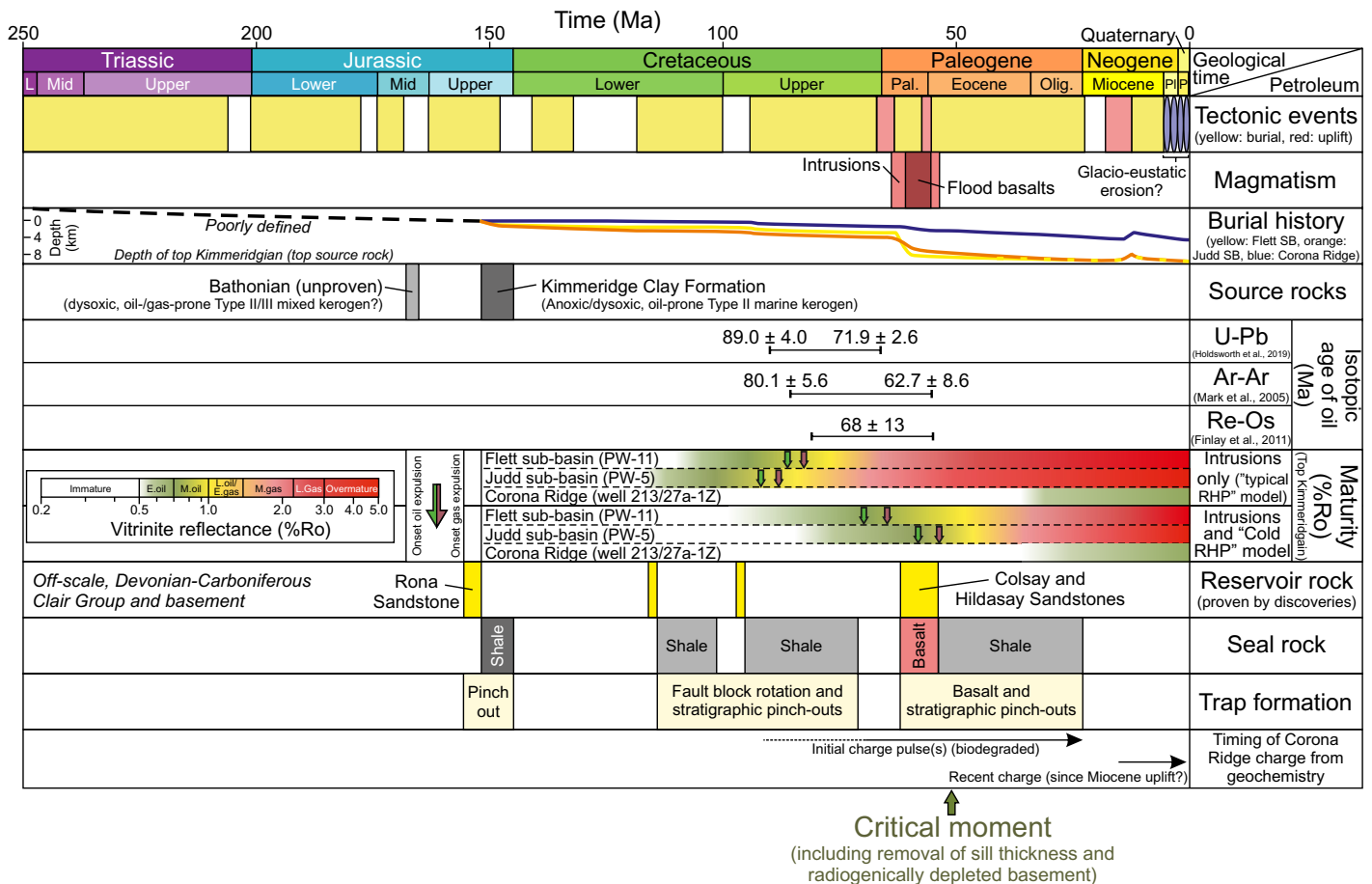


Figure 3. Petroleum systems chart (PSC) for the Faroe-Shetland Basin (FSB; offshore UK) integrating source, reservoir, seal, and trap components of the Mesozoic to Paleogene petroleum system. A comparison of published geochemically constrained charge timing estimates from oils and petroleum inclusions within the FSB, using U-Pb (Holdsworth et al., 2019), Ar-Ar (Mark et al., 2005), and Re-Os (Finlay et al., 2011) isotopic dating, with findings of this study shows good correlation to the predicted oil generation age in the center of the source-rock kitchens (areas of subsidence where source rock has reached appropriate conditions of pressure and temperature to generate liquid hydrocarbons) (Flett and Judd sub-basins [SBs]) using just intrusions with radiogenic heat production (RHP) of 2.8 μW/m³ (akin to the North Sea) (“the typical RHP” model) and the same intrusion model using the “cold RHP” model (with a lower RHP of 1.6 μW/m³ calculated from basement samples of Neoproterozoic orthogneisses from wells 204/10-1 (Amerada Hess Corporation, 2002), 205/16-1 (BP, 1986) and 214/9-1 (Total, 2000). Maturity reference modeled well on Corona Ridge, 213/27a-1Z drilled by Texaco in 2004. PW—pseudo-wells (as shown in Figure 1). L—Lower; Mid—Middle; Pal.—Paleocene; Olig.—Oligocene; Pl.—Pliocene; P—Pleistocene; E.—early; M.—main; L.—late; Sst.—Sandstone.

system. This should be considered carefully on a sub-basin scale.

2. The consideration of the increase in thermal conductivity that results in a sedimentary unit when more thermally conductive igneous rock is intruded into the less thermally conductive sediment.
3. The use of correct basement composition, age, and RHP (calculated locally where possible), particularly in areas of ancient basement where RHP can be significantly lower than assumed values.

Although our study is focused on the FSB, our findings apply to any sedimentary basin in which considerable intrusive igneous activity exists (e.g., the northwestern shelf of Australia, South Atlantic margins, and North Atlantic margins) or where basement composition varies. This work has potentially wider implications outside of petroleum exploration, including geophysical and stratigraphical interpretations and overestimation of crustal stretching (β -factor [the ratio of final lithospheric thickness to original lithospheric thickness]) in passive margins based on sediment thickness.

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