



1 **Thrusts control the thermal maturity of accreted sediments**

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Abstract.

Thermal maturity assessments of hydrocarbon-generation potential and thermal history rarely consider how upper-plate structures developing during subduction influence the trajectories of accreted sediments. Our thermomechanical models of subduction support that thrusts evolving under variable sedimentation rates and décollement strengths fundamentally influence the trajectory, temperature, and thermal maturity of accreting sediments. This is notably true for the frontal thrust, which pervasively partitions sediments along a low and a high maturity path. Our findings imply that interpretations of the distribution of thermal maturity cannot be detached from accounts of the length and frequency of thrusts and their controlling factors. Taking these factors into consideration, our approach provides a robust uncertainty estimate in maximum exposure temperatures as a function of vitrinite reflectance and burial depth thereby reducing former inconsistencies between predicted and factual thermal maturity distributions in accretionary wedges.



1. Introduction

Organic material transforms into coal, oil, and gas at rates primarily controlled by temperature (Quigley & Mackenzie, 1988). This transformation, critical for the hydrocarbon industry, is also useful to study the tectonic and sedimentary evolution of basins and orogens (Tissot et al., 1987; Tissot & Welte, 2013; Waples, 1981). The extent of this transformation in sediments, known as thermal maturity, can be measured as vitrinite reflectance; the percentage of incident light reflected from the surface of vitrinite particles in those sediments (Burnham & Sweeney, 1989). Thermal maturity has been used to estimate the thermal evolution of igneous intrusions (Bostick & Pawlewicz, 1984) and seismic slip (Rabinowitz et al., 2020), the extent of diagenesis and low-grade metamorphism (Ferreiro Mählmann & Le Bayon, 2016; Totten & Blatt, 1993), porosity and compaction in basin sediments (Schmoker & Gautier, 1988), as well as the geothermal history of accreting material during subduction (A. Sakaguchi et al., 2011; Underwood et al., 1992; Yamamoto et al., 2017).

Inferences on the geothermal history of subduction margins based on thermal maturity depend on the trajectory followed by the accreting sediments (Miyakawa et al., 2019). Low-temperature high-pressure metamorphic rocks in the subduction wedge are often attributed to the pressure maxima that typically predate the temperature maxima **in sediments accreted in the wedge** (Platt, 1993). However, numerical models (Ruh, 2020b) and field observations (Giunchi & Ricard, 1999) have indicated the existence of complicated patterns in sediment trajectories. As ~~the orogenic~~ wedge evolves, sediments accreting along different paths reach different depths and velocities and are exposed to different regional peak temperatures. Miyakawa (2019) proposed to subdivide these trajectories based on their final characteristics such as thermal maturity. As a result, the spatiotemporal evolution of the sediments which regulate thermal maturity is controlled, to a first-order, by the partition of incoming sediments along two end-member pathways; (i) a deeper path leading to elevated thermal maturities, the **high thermal-maturity path**, and (ii) a shallower path resulting in low thermal maturity, the **low thermal-maturity path** (Miyakawa et al., 2019).

Although a number of researchers have studied the diversity of particle paths by their Pressure-Temperature evolution in accreted and underthrust sediments, ~~in presence of~~ surface processes, distribution of surface processes, in both analytical and numerical models (Hori & Sakaguchi, 2011; Elena Konstantinovskaia & Malavieille, 2005; Platt, 1986; Ruh, 2020a; Wenk & Huhn, 2013), its correlation or lack thereof with its pre-accreted state has not been suitably investigated. Much remains to



76 be explored regarding how the partition of high/low thermal maturity paths and the general translation of sediments occurs
 77 inside the wedge, given the conventional assumption that accreting sediments remain at the same relative depth (Hori &
 78 Sakaguchi, 2011) and translate along the adjacent “layers” without vertical mixing throughout the tectonic evolution of the
 79 wedge (Luján et al., 2010; S. Willett et al., 1993) to yield this diversity of sediment paths. To better understand the time-depth
 80 paths of wedge sediments, their dependence on the initial state of undeformed sediments, and thus their thermal maturity, the
 81 factors that control the evolution of subduction-accretion systems, like sedimentation, erosion, and décollement strength
 82 (Mannu et al., 2016; Simpson, 2010), ought to be considered.

83 Here, we explore in detail the impact that a realistic account of accretion in a subduction wedge has on the thermal
 84 maturity of its sediments. We simulate subduction-accretion using 2D finite-difference thermomechanical models
 85 incorporating empirical thermal conductivity values from the Nankai accretionary margin. We track the evolution of thermal
 86 maturity by computing vitrinite reflectance(%R₀) using three well-established methods of %R₀ computation, ~~on each marker~~
 87 ~~in the model~~ as the wedge develops by accretion under different sedimentation rates and décollement strengths. ~~These factors~~
 88 ~~notably alter the trajectories and thermal maturities of incoming sediments.~~ Particularly, thrusts define sharp thermal maturity
 89 boundaries leading to ~~stark differences~~ in the thermal maturity of sediments that accrete in different thrust blocks, even when
 90 they follow similar trajectories and lay nearby.

91

92 2. Methods

93 We employ I2VIS, a conservative (Gerya, 2019) finite-difference 2-D thermomechanical ~~subduction-accretion model~~ with
 94 visco-plastic/brittle rheology (Gerya & Yuen, 2003). The code solves the governing equations for the conservation of mass,
 95 momentum, and heat as well as the advection equation with a non-diffusive marker-in-cell scheme (Gerya, 2019) constrained
 96 by thermal conductivity values inferred from Nankai accretionary wedge (Sugihara et al., 2014). Our numerical approach has
 97 several advantages over earlier models to simulate thermal maturity in an accretionary wedge(Miyakawa et al., 2019), such as
 98 a more realistic geothermal profile, variable particle paths, and thermal evolution. The supplementary material contains
 99 information regarding the governing equations, the modified thermal conductivity formulations based on the C0002 borehole



in the Nankai accretionary wedge, boundary conditions, the rheological model, model setup (Fig S1) and surface processes (Fig S2).

2.1 An improved thermal maturity calculation

Given that assessments of thermal maturity are inherently reliant on the distribution of temperature inside the wedge, any attempt to model thermal maturity needs a realistic temperature gradient in the wedge. We incorporate this by modifying the thermal conductivity computation for sediments and décollement (see Table 1 and section 1 in the provided supplementary text) to match the empirical relationship between depth and thermal conductivity, as measured on core samples in the borehole IODP Site C0002 (Sugihara et al., 2014; Tobin et al., 2015). Both for the same accretionary wedge is scarce to find, and to our knowledge, the C0002 borehole in Nankai accretionary wedge along the Kumano forearc basin is the only place with available datasets for both thermal conductivity and thermal maturity values for an accretionary wedge (Fukuchi et al., 2017). The model computes the %R₀ of each marker to estimate the thermal maturity of sediments during the model run using three widely used methods of thermal maturity modelling Easy%R₀ (Burnham & Sweeney, 1989), Simple%R₀ (Suzuki et al., 1993) and Basin%R₀ (Nielsen et al., 2017). All these approaches for computing %R₀ yield similar trends albeit different absolute values. In the interest of clarity, we have mostly illustrated Easy%R₀, which is the most extensively used method for Vitrinite Reflectance computation. Hence, in the interest of clarity, we have mostly illustrated Easy%R₀, which is the most extensively used method of Vitrinite Reflectance computation. Hence, hereafter we refer Easy%R₀ as simply %R₀, unless explicitly stated. %R₀ is set to 0.2 in sediment markers at the start of the model till 2.5 Myr, while %R₀ in markers for other rocks, air, and water is undefined at all times. After 2.5 Myr, the model computes %R₀ on each marker as a function of temperature (T), time (t), and amount of fixed carbon as a percentage (f_c). The initial %R₀ of newly deposited sediments is computed using an assumed water-sediment interaction temperature assumed to be the same as the thermocline. The thermocline used in the model has been estimated using the data obtained and made freely available by International Argo Program and the national programs that contribute to it for the region near Nankai (Argo, 2022). is set to 0.2 in sediment markers at the start of the model till 2.5 Myr, while %R₀ in markers for other rocks, air, and water is undefined at all times. After 2.5 Myr, the model computes %R₀ on each marker as a function of temperature (T), time (t), and amount of fixed carbon as a percentage (f_c). The initial %R₀ of newly deposited sediments is computed using a water-sediment interaction temperature assumed to be the same as the



thermocline. The thermocline used in the model has been estimated using the data obtained and made freely available by International Argo Program and the national programs that contribute to it for the region near Nankai (Fig S3, Argo, 2022).

2.2 Experimental Strategy

Here, we present a total of 10 models that vary in their effective basal friction or their effective sedimentation rate to discern patterns of thermal maturity evolution in wedge sediments. Models M_0^2 , M_0^7 , M_0^{12} , M_0^{17} , M_0^{22} , have no sedimentation and effective internal angle values for the décollement of $\phi_b = 2^\circ, 7^\circ, 12^\circ, 17^\circ$ and 22° respectively. The chosen range of effective décollement strength is well within the range of values postulated by several studies for the Nankai accretionary wedge (Tesei et al., 2015). The rest of the models shown here, $M_{0.1}^{12}$, $M_{0.3}^{12}$, $M_{0.5}^{12}$, $M_{0.7}^{12}$, and $M_{0.9}^{12}$ have a medium-strength décollement and variable effective sedimentation rate ranging from 0.1 to 0.9 mm/yr. Sedimentation occurs only at the trench in all of the models presented in this study from sea to land. With these models, we evaluate the particle trajectory and %R₀ of accreting sediments as a function of décollement strength (M_0^2 - M_0^{22}) and sedimentation rate ($M_{0.1}^{12}$ - $M_{0.9}^{12}$). To restrict the number of parameters influencing our observations, models have no erosion. Moreover, all models lack surface processes during the first ~2.5 Myr and have sedimentation thereafter. Sediments used in the model have an angle of friction of 30° and a strain-softened value of 20° after a threshold of 0.5-1.5 strain. The coefficient of friction increases linearly between the thresholds. Sedimentation rates are the effective sedimentation rate computed after the model run and are thus not prescribed a priori. This choice ensures that the range of average sedimentation in all our models (0.1-0.9 mm/yr) lies within observed sedimentation rates in our chosen natural equivalent, the Nankai accretionary wedge in the south-western subduction margin of Japan (Korup et al., 2014). Table 2 provides more details about the model run and prescribed sedimentary conditions.

3. Results

Subduction begins at 0.1 Myr as the weak material between continental and oceanic plate fails (see supporting information movies). Continued and sustained accretion of sediments against the deforming continental crust forms the accretionary wedge from the interplate contact landwards. After ~5 Myr, all models develop a distinct wedge in agreement with the critical taper theory (Davis et al., 1983). Taper angles increase systematically as effective basal friction increases from $\sim 2^\circ$ to $\sim 22^\circ$ (Fig 1, Table 2, $M_0^2 - M_0^{22}$). Whereas models with a relatively weaker décollement, as M_0^2 ($\phi_b = 2^\circ$), have taper slopes of $4.3^\circ \pm$



0.3°, models with very strong décollement, as M_0^{22} ($\phi_b = 22^\circ$), have slopes as steep as $12.8 \pm 1.2^\circ$ (Table 2). Models without trench sedimentation grow solely by accretion of incoming seafloor sediments, with frequent nucleation of frontal thrusts. Models with weaker décollements develop thrusts that are lengthier and remain active for shorter periods. This is clear when comparing, for models with increasingly strong décollement $M_0^2 - M_0^{22}$, the average distance between first and second frontal thrusts are 15.5 ± 7.0 km, 12.1 ± 3.6 km, 8.8 ± 3.3 km, 8.7 ± 2.1 km and 8.0 ± 1.8 km, respectively. Increasing sedimentation rate also leads to an increase in thrust sheet length from 7.3 ± 1.1 km in $M_{0.1}^{12}$ to 13.8 ± 7.8 km in $M_{0.9}^{12}$. In models with similar basal friction, models with higher sedimentation rates have lengthier thrust sheets that remain active for longer periods (Table 2). Steeper surface slopes with increased décollement strengths and change in thrust sheet length with sedimentation and décollement strength are well-known effects that have been confirmed by previous numerical (Mannu et al., 2016; Wang & He, 1999) and analytical (Malavieille & Trullenque, 2009; Storti & McClay, 1995) models. All the reported values are mean \pm Standard Deviation values recorded between 2.5-7.5 Myr in individual models. All models, exhibit a temperature gradient that corresponds well with the temperature profile observed in the boreholes at IODP Site C0002 in the Kumano forearc basin, on top of the Nankai accretionary wedge (Fig. S4).

3.1 Thermal maturity of the wedge

Sediments are more thermally mature in wedges that have a higher sedimentation rate or décollement strength. For example, the mean %R₀ of simulations for wedges with the highest sedimentation ($M_{0.9}^{12}$) is 12% higher (0.75) than in those without sedimentation (M_0^2) (Table 2, Fig 1). Similarly, simulations of wedges with the strongest décollement have the highest mean %R₀ (0.94) of all the simulations presented in this study.

Thermal maturity values increase with depth and landward distance from the trench to the forearc high irrespective of the décollement strength, sedimentation rates and method of thermal maturity computation (Fig. 1). As a result, sediments at the core of the wedge consistently reach the highest maturity. The absolute value of %R₀ and the rate at which thermal maturity values increase landward from the trench are larger for wedges with high décollement strength (Fig. 2A). In wedges with the same décollement strength but higher trench sedimentation the rate of thermal maturity increase landward from the trench remain very similar (Fig. 2B). Comparing the values of %R₀ (Fig. 2) along an arbitrary horizon in several models



emphasizes this result; the model with the highest décollement strength attains the maximum $\%R_0$ of 1.25, and has the highest rate of landward increase in thermal maturity (Fig. 2A). However, all models with similar décollement strength but different sedimentation do not visibly vary in their rate or magnitude of landward increase in thermal maturity. All models show a decrease in thermal maturity landward of the forearc high, commonly of 0.2 $\%R_0$. Other interesting observations that we explore below are the increased thermal maturity occurring in the vicinity of thrusts (e.g. Fig 1) and the reversal in sediment maturity around out-of-sequence thrust (e.g. Fig 1) active over longer times visible across several models (Fig 1).

The magnitude of $\%R_0$ varies consistently among Easy $\%R_0$, Simple $\%R_0$ and Basin $\%R_0$. On average Easy $\%R_0$ have the smallest values, followed very closely by Basin $\%R_0$ (with an average difference of only 0.02). However, Simple $\%R_0$ had the highest average value of thermal maturity being 0.16 and 0.13 higher than Easy $\%R_0$ and Basin $\%R_0$ (Fig 1).

3.2 Sediment trajectory inside the wedge

Sediments follow high-maturity paths in larger proportions in wedges with a higher décollement strength or sedimentation rate. We demonstrate this effect by creating a map of the thermal maturity of sediments at 7.5 Myr of the model run, mapped to their spatial position 5 Myr earlier (at 2.5 My of the model run) (Fig. 3) to analyse the spatial correlation between sediment position (depth and distance) from the trench and thermal maturity. We also show the mean thermal maturity attained by sediments at a given horizontal distance from the trench during this period. The scatter plot shows sharp changes with distance from the trench that relate to changes in sediment trajectory (Fig. 3). The mean thermal maturity is also variable along the horizontal length of the wedge and has a periodicity increasing in distance with higher sedimentation rate but relatively constant with changing basal friction (Fig. 3). Whereas the mean thermal maturity has a short periodicity of ~7.2 km for the model M_0^{12} with no sedimentation rates, the model $M_{0.9}^{12}$ shows the longest periodicity of 21 km. However, for all models with the same no sedimentation M_0^2 - M_0^{22} the periodicity remains relatively consistent between the range of 7-8 km.

Fig 3 also represents the distribution of trajectories that exist in an accretionary wedge and how these trajectories get impacted under trench sedimentation (a subset of these trajectories can be viewed in the supplementary Fig. S5). Whereas in wedges with weak décollements (M_0^2), none of the shallowest half of incoming sediments reach $\%R_0 > 1$ in 5 Myr, 2% of



sediments reach this value in wedges with strong décollement (M_0^{22}). The effects of décollement strength in the thermal maturity of sediments can be quantified as well at deeper levels, with one-eighth vs more than half of the sediments surpassing values of $\%R_0 = 1$ for the deepest half of incoming sediments (12.0% and 54% respectively) in weak vs strong-decollement wedges (M_0^2 vs M_0^{22}), respectively. Increasing the sedimentation rate shows this effect even more prominently. In wedges from the model without sedimentation (M_0^{12}), none of the top half m of sediments yield $\%R_0 > 1$, while ~ 15% of them surpass $\%R_0 > 1$ in the models with a sedimentation rate of 0.9 mm/yr ($M_{0.9}^{12}$). In sum, the proportion of sediments in the top half and bottom half of the wedge that reach high maturity steadily increases with both sedimentation rate and décollement strength (Table 2).

3.3 Patterns of trajectory and thermal maturity in incoming sediments

The diversity in the trajectory of sediments in the wedge leads to a plethora of pathways in which the sediments can become thermally mature and thus introduces epistemic uncertainty in the estimation of maximum exposure temperature. Fig 4, captures this uncertainty where we plot the maximum exposure temperature as a function of $\%R_0$ for all the models simulated in this study. We find that almost all the models show a remarkable similarity in their relationship between maximum exposure temperature and $\%R_0$ (for individual models please see Fig S6) and differ mostly in their proportion of sediments with extreme values of $\%R_0$. We observe that the typical uncertainty in maximum exposure temperature increases with an increase in values of $\%R_0$ with ~ 15°C interval at around $\%R_0=0.2$ compared to ~33°C interval at $\%R_0= 3$ (both for 95% confidence interval, Fig. 4b). Furthermore, we observe that information about the present depth of the sediments w.r.t the thickness of the wedge (as represented by different colours in Fig 4a) greatly helps to further constrain the maximum exposure temperature. For instance, although the overall uncertainty at $\%R_0=1$, is ~23°C, for sediments with a normalized depth of 0.2-0.4, the uncertainty greatly reduces to only ~10.5°C. Thus the range of thermal maturity values for sediments clearly has a large correlation with their trajectories.



3.4 Comparison of Easy% R_0 , Simple% R_0 and Basin% R_0

Finally as our models produced three sets of % R_0 using Easy% R_0 (referred to as $R_0\%$ throughout our study-), Simple% R_0 and Basin% R_0 , it also gives us a unique perspective on comparative advantages of each method. Uncertainty for all three models increases with increasing % R_0 from ~20–25°C at ~0.3 which rises to ~35°C at $R_0\%=3.5$ (Fig 4b). Easy% R_0 is the most well-recognised method of thermal maturity computation and yields the best constraint on uncertainty for very small changes around the values less than 1. For the values of % R_0 between 1 and 3, all models yield very similar uncertainty, with Simple% R_0 yielding the most constrained exposure temperatures (Fig 4b). However, beyond $R_0\%=3$, the Simple% R_0 becomes highly unreliable, with uncertainty in exposure temperatures as high as 55°C at $R_0\%=4$. Easy% R_0 yields a reasonable uncertainty range of ~37°C till $R_0\%=4.4$, but starts to be unreliable above this value. Basin% R_0 remains consistent till a very high value of $R_0\%$ (~6), and thus provides the best constraint on the widest range of values of thermal maturity (Fig 4b).

4. Discussion

Our models achieve realistic thermal maturity distributions thanks to unique computational advantages over models in the previous studies (Mannu et al., 2016, 2017; Miyakawa et al., 2019), despite several relevant assumptions. Models are simplified by assuming no elasticity, predefined décollement, no erosion, and using simple and uniform rheology, and either has an insufficient resolution or lack empirical relations to simulate the compaction of sediments and processes of multiscale fluid flow. Although these assumptions hinder a wholesale comparison between our simulations and natural examples of accretionary wedges, we are confident of the thermal maturity patterns of our models. Our estimated % R_0 values for the model $M_{0.1}^{12} - M_{0.9}^{12}$ are in very good agreement with the % R_0 values measured for the borehole C0002 Nankai accretionary wedge (used for thermal conductivity values) by Fukuchi et. al. 2009 (Figure 5). Moreover, the temperature estimated from the observed thermal maturity of a timeframe of 1-2 Myr in the borehole, also strongly correlates with the trend and the range of 95% Confidence interval of T vs % R_0 estimated in our models (Fig S7). Furthermore, our models also correlate with the patterns of P-wave velocity for Nankai (Górszczyk et al., 2019; Nakanishi et al., 2018) and Hikurangi (Arai et al., 2020) margins (Dewing & Sanei, 2009). Models compute realistic thermal maturity distributions thanks to several key improvements.



241 Firstly, our models calculate temperature gradients that evolve at long time intervals and thus closely replicate **accretionary**
 242 **wedges in nature** (Fig. S2). This enables the simulation of realistic temperature profiles based on thermal conductivity values
 243 derived empirically from natural accretionary wedges, as in our case, the Nankai margin (Sugihara et al., 2014). Secondly, our
 244 simulations account for the effects that thermal and isostatic feedback from the oceanic lithosphere have on the evolution of
 245 the wedge by simulating plate subduction at a large scale rather than just the accretionary wedge (Miyakawa et al., 2019).
 246 Finally, our method calculates the vitrinite reflectance of sediments on each marker of the model. This capacity to accurately
 247 estimate thermal maturity in **each marker informs** the research questions of this study and allows inferences beyond those of
 248 depth-dependent thermal maturity distributions.

249 The thermal maturity of the wedge increases landward, as signalled by the landward increase in %R₀ (Fig. 1). This
 250 has been observed in natural accretionary wedges such as Miura–Boso plate subduction margin (Yamamoto et al., 2017), fold
 251 **and thrust belts Western Foothills complex in western Taiwan** (Arito Sakaguchi et al., 2007) and **other numerical models of**
 252 **accretion** (Miyakawa et al., 2019), resulting from the long-term deformation of older accreted sediments and the backstop-
 253 forced exhumation in the wedge. Our models show that the rate of landward rise in thermal maturity is faster for thicker wedges
 254 (Fig 2). This is the case for wedges with high basal strength (M_0^{22}), **for sediments in thicker wedges deform more prominently**
 255 **than those in their thinner counterparts**. Simulations also show that **sediments reach deeper levels in thicker wedges and that**
 256 **this increases the overall thermal maturity of the wedge**. Also, increased exhumation rates and steeper thermal maturity
 257 gradients occur in the wedge interior, as the continental backstop deflects sediment trajectories upwards during accretion (Fig.
 258 2). As a result, for the **geometry of the backstop used in our models**, backstop-forced exhumed material is, on average,
 259 thermally more mature.

260 Our models expose two relevant cases where the increase of thermal maturity with depth or landward is relevantly
 261 altered: on-fault increase and fault-block inversion. Our models attest to the steep rise in thermal maturity of sediments at fault
 262 sites (Fig. 1). This is **well documented in** nature, as for boreholes C0004 (Sakaguchi et al., 2011). However, on-fault increases
 263 in thermal maturity are comparatively smaller in our simulations and lack the marked increase in %R₀ observed at fault sites
 264 in nature. **This is primarily due to our models developing wider fault zones than their natural equivalents and the subsequent**
 265 **acceleration in the thermal diffusion occurring in simulated thrusts**. During fault-block inversions, the positive gradient of



thermal maturity with depth is inverted by thrusting relatively mature sediments over less mature sediments (Underwood et al., 1992). This is known from natural observations, as along the Fukase Fault in Shimanto accretionary wedge (Ohmori et al., 1997) and underneath the forearc basin in Nankai accretionary wedge (Fukuchi et al., 2017), and previous modelling efforts (Miyakawa et al., 2019).

Collation of the above implies that the thermal maturity of accretionary wedges results from the general increase of thermal maturity (i) with depth and (ii) landward, as well as from its (iii) modification by thrust faults. Our models suggest thermal maturity inversions by thrusting, which are commonplace in accretionary contexts, are the primary cause of thermal maturity differentiation among wedges with initially similar geothermal gradients. In other words, the strong differentiation in the trajectory of sediments led by thrusting has a larger influence over thermal maturity than burial depth or in-wedge location. This novel inference has probably remained concealed thus far due to the large number of parameters that condition thrust development, frequency, length, and thermal state. Influencing parameters to include sedimentation, erosion, basal friction and relief, pore pressure and fluid state, wedge length and thickness, taper angle, and many others (Dominguez et al., 2000; E. Konstantinovskaia, 2005; Mannu et al., 2016; Ruh, 2017; Simpson, 2010; H. J. Tobin & Saffer, 2009). It is nevertheless important to note that the frequency of faults in a wedge can be impacted by many other factors, including hinterland sedimentation (Simpson, 2010; Storti & McClay, 1995), erosion (E. Konstantinovskaia, 2005; S. D. Willett, 1999), and seafloor topography (Dominguez et al., 2000). Below, we discuss how thrusts not only alter the thermal evolution of accreting sediments but are, in fact, the primary control of their thermal maturity.

Thermal maturity correlates with sediment depth weakly near faults and more strongly away from them. The distance of sediment from frontal thrust dictates the trajectory of sediment grains, and as a result, the pressure-temperature conditions to which they are exposed. In this study, we have considered solely how décollement strength and the rate of trench sedimentation vary the frequency, architecture, and overall behaviour of thrusts, and the frontal thrust, as the wedge evolves. Our results show the need to consider all factors influencing fault frequency when inferring the geothermal history of contractional terrains by means of thermal maturity. Fortunately, this predictive exercise should be relatively straightforward, for the impact of these external factors on the fault structure of wedges has been established (Fillon et al., 2012; Mannu et al.,



2016, 2017; Mugnier et al., 1997; Simpson, 2010; Storti & Mcclay, 1995), and the effect of each of these factors can be accounted for when assessing the trajectory of sediments and the distribution of thermal maturity in accretionary wedges.

Sediment mixing in subduction wedges is primarily controlled by thrusting. Previous studies have reached seemingly contradicting outcomes when using numerical (Miyakawa et al., 2019; Wenk & Huhn, 2013; S. Willett et al., 1993) and analogue (E. Konstantinovskaia, 2005; Mulugeta & Koyi, 1992) approaches to analyze sediment trajectories as a function of changes in erosion, sedimentation, or décollement strength. While some studies showed that the rate and extent of a transition by which sediment trajectories change from generally horizontal to increasingly vertical during accretion change consistently with the initial depth of incoming sediments (Mulugeta & Koyi, 1992; S. Willett, 1992), others predicted different crossover paths for sediments accreting over a range of décollement strengths (E. Konstantinovskaia, 2005). Our models show that both are valid results and that changes in trajectory patterns leading to path crossovers are controlled by the horizontal distance of sediments from the frontal thrust. Starting at a threshold distance from the trench, sediments at different depths follow laminar paths along different trajectories within the wedge. Laminar-type trajectories can be reproduced in a broad range of simulations and are particularly common in models with low sedimentation and décollement strengths. However, the depth dependence of sedimentary paths varies periodically as a function of distance from the trench of specific sedimentary packages (Fig. 3,6). This effect, which is particularly marked in the neighbourhood of the frontal thrust, explains the crossover paths for incoming sedimentary packages at similar depths and different horizontal locations, as shown by Konstantinovskaia et al. 2005. Therefore, thrust faults in the wedge act as the primary agent controlling whether sediments sustain depth-controlled laminar flow or mix.

The thermal maturity that incoming sediments reach varies periodically as a function of thrust frequency. Although previous research considered non-laminar sediment trajectories as chaotic (Mary et al., 2013), and the wide variety of trajectories shown in our models seem to agree with this (Fig 3, Fig S4), patterns emerge when we correlate the lateral and vertical position of incoming sediments with their eventual thermal maturity. Changes in the depth of the thermal maturity boundary are less frequent and have larger amplitudes with increased décollement strength, and especially, increased sedimentation rates (Fig. 4). The periodicity in the thermal maturity boundary marks the periodic oscillation of the predominant trajectory followed by incoming sediments, i.e., between accretion (low thermal maturity path) and underthrusting (high-



thermal maturity path). As a result, it should also strongly correlate with the periodicity observed in the evolution of forearc topography (Menant et al., 2020) and the frequency of thrust formation as such in our models. This is expected, given that thrusts are active over longer mean times, and they thus channel material toward the décollement more efficiently, in wedges with stronger décollement or increased sedimentation. While sediments at internal and higher structural positions of the wedge are translated towards the surface and have a lower thermal maturity, sediments at external and lower structural positions are translated towards the décollement and have a relatively higher maturity. This is a relevant observation, for it typifies the causality of particular sediment grains following a high or low maturity path, a long-standing unanswered question (Miyakawa et al., 2019). We corroborate this observation by analyzing the terminal thermal maturity of sediments across a frontal thrust active at a younger age. For example, by showing the thermal maturity of sediments at ~7.5 Myr across a thrust active at ~4 Myr, as in Fig. 7. Whereas this occurs for all thrusts in the wedge, the frontal thrust is particularly pronounced in partitioning sediments into the high and low maturity paths.

Geothermal information stored in the incoming sediments can only be retrieved if sediments are at appropriate locations with respect to emergent thrusts. We illustrate this using two runs of the same model and tracking an artificial thermal anomaly imposed on incoming sediments at two different locations (Fig. 7). This hypothetical thermal anomaly can be conceptualized as any alteration of the thermal maturity profile of incoming sediments, for example, elevated heat flows by an antecedent magmatic intrusion. While the change in %R₀ associated with the short-lived thermal anomaly results in abnormally high values of thermal maturity in both sediment packages, it can only be retrieved for the end-model run of sediments located further from the trench (those in the right panel, Fig. 7b). Contrarily, the end-model run of sediments closer to the trench (those in the left panel, Fig. 7a) shows no signs of discontinuity in the thermal maturity distribution of the wedge. This is because we deliberately placed the thermal anomaly at sites that evolve at two structural locations during the model run, i.e., above and below a yet-undeveloped frontal thrust (Fig. 7). The sediment sector affected by the thermal anomaly closer to the trench is overthrust by the frontal thrust and remains in a footwall location thereafter (Fig. 7a). In contrast, the homologous sedimentary package further away from the trench is accreted by the frontal thrust and remains in a hanging-wall location (Fig. 7b). Thus, the preservation of the record of an antecedent thermal anomaly is only possible in the former case. We further note that, in our simulations, the entire vertical column of sediments records the thermal anomaly, while in nature, the anomaly may



340 affect only sediments at the deeper locations of the sedimentary pile, which are in turn the sediments that most likely to follow
341 a high-maturity path. We thus regard the possibility of retrieving such antecedent geothermal information as minimal.

342 The main implications of this contribution emerge from its predictive power. Our approach can predict to a precise the thermal
343 maturity of sediments and the uncertainty associated with the maximum exposure temperature in accretionary contexts with
344 known structuration. More accurate quantification of the thermal evolution and thermal state of accreted sediments reduces
345 the uncertainties attached to the location of temperature-led transformations of organic material into hydrocarbons in
346 subduction margins and other accretionary contexts. Such increased accuracy in the distribution of thermally mature sediments
347 may also be applied for improved assessments of the evolution in time of any other geothermal process, including seismic slip,
348 magmatic and metamorphic extent, porosity, compaction and diagenesis of sediments, and the reconstruction of convergent
349 margins in general (Bostick & Pawlewicz, 1984; Ferreiro Mählmann & Le Bayon, 2016; Rabinowitz et al., 2020; A. Sakaguchi
350 et al., 2011; Totten & Blatt, 1993; Underwood et al., 1992).

351 Finally, among the three methods of $\%R_0$ computation, Easy $\%R_0$ and Basin $\%R_0$ are clearly more consistent and well-
352 constrained on a wide range of thermal maturity in comparison to Simple $\%R_0$, which seems to be particularly useful for a
353 smaller range of thermal maturity values. This simply illustrates the fact that while Easy $\%R_0$ and Basin $\%R_0$ computation
354 deals with several parallel reactions related to the maturity of kerogen (and hence multiple activation energies), the Simple $\%R_0$
355 is based on best-fitted single activation energy, and hence yields large confidence intervals at the extreme $\%R_0$ values.
356 Additionally, the inclusion of the higher activation energy reactions in Basin $\%R_0$ makes it the best-suited formulation for
357 sediments at the deeper and shear zone sediments which usually get saturated using Easy $\%R_0$.

358 4. Conclusion

359 This study demonstrates how contractional faults alter the paths of sediments as they accrete and how this fundamentally
360 controls the distribution of the thermal maturity of sediments in accretionary wedges and emphasizes the role that
361 sedimentation rate and interplate contact strength have in such distribution. The increased resolution of our approach leads to
362 findings that have relevant implications. For example, the geothermal history that can be retrieved from the thermal maturity
363 of sediments in drills, i.e., at the shallow wedge, provides, at best, an incomplete record that is skewed towards the thermal



evolution of sediments near the trench. Coevally, relevant sectors of sediments located further seaward, when not subducted, follow high-maturity paths that overprint their antecedent thermal history. Finally, this study also provides a first-order uncertainty measure for the thermal maturity of sediments based on the diversity in their trajectory.

Competing interests

The authors declare that they have no conflict of interest.

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Table 1: Properties for the different materials used for the model runs

Rock Type	Density (kg/m ³)	Cohesion (MPa)	Coefficient of friction(μ)	Thermal Conductivity (W/(m K))	Flow law	E (kJ/mol)	n
Water	1000	0	0	20		0	0
Air (Sticky-air)	0	0	0	20		0	0
Décollement	2600	0.001	0.03 / 0.08	$(1.5+807/(T+77))^* (1-\exp(-Z^2/1.3e7))$	Wet quartzite	154	2.3
Sediments1	2600	0.5/0.05*	4.64/0.2*	$(0.96+807/(T+77))^* (1-\exp(-Z^2/1.3e7))$	Wet quartzite	154	2.3



Sediments2	2600	0.5/0.05*	4.64/0.2*	$(0.96+807/(T+77))^* (1-\exp(-Z^2/1.3e7))$	Wet quartzite	154	2.3
Upper Continental Crust	2700	1	0.6	$0.64+807/(T+77)$	Wet quartzite	300	2.3
Lower Continental Crust	2800	1	0.6	$0.64+807/(T+77)$	Wet quartzite	300	3.2
Upper Oceanic Crust	3000	1	0.6	$1.18+474/(T+77)$	Plagioclase An75	300	2.3
Lower Oceanic Crust	3000	1	0.6	$1.18+474/(T+77)$	Plagioclase An75	300	3.2
Mantle Lithosphere	3300	1	0.6	$0.73+1293/(T+77)$	Dry olivine	532	3.5
Asthenosphere	3300	1	0.6	$0.73+1293/(T+77)$	Dry olivine	532	3.5
*Strain-softened Cohesion/Coefficient of friction T is Temperature, Z is the depth from the seafloor.							

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510



511 **Table 2: Model runs and their specific characteristic observations**

Models	φ_b	φ / φ_{ss}	SR	L	α	D	$\langle R_o \% \rangle$	% _{top-half}	% _{Bottom-half}
M_0^2	2°	30°/15°	None	123.2±15.7	4.3±0.3°	15.5±7.0	0.54	0.0	12.7
M_0^7	7°	30°/15°	None	97.7±9.9	6.5±0.5°	12.1±3.6	0.60	0.0	22.5
M_0^{12}	12°	30°/15°	None	77.8±4.8	8.9±0.5°	8.7±2.1	0.67	0.0	31.3
$M_{0.1}^{12}$	12°	30°/15°	0.1	76.1±5.9	8.9±0.9°	7.3±1.1	0.71	0.1	35.3
$M_{0.3}^{12}$	12°	30°/15°	0.3	79.3±8.2	8.6±1.3°	7.8±2.5	0.69	0.1	32.0
$M_{0.5}^{12}$	12°	30°/15°	0.5	79.9±7.4	8.5±0.6°	9.5±4.0	0.71	2.7	34.4
$M_{0.7}^{12}$	12°	30°/15°	0.7	81.3±10.5	8.5±1.0°	9.9±5.0	0.73	4.2	41.5
$M_{0.9}^{12}$	12°	30°/15°	0.9	82.5±11.0	8.8±1.5°	13.8±7.8	0.75	14.6	51.8
M_0^{17}	17°	30°/15°	None	71.6±5.0	10.7±0.8°	8.8±3.3	0.83	1.2	40.6
M_0^{22}	22°	30°/15°	None	62.7±6.0	12.8±1.2°	8.0±1.8	0.94	2.0	54.0

φ_b is décollement Strength (internal angle of friction)

φ Sediment Strength

φ_{ss} Sediment Strength (Strain weakened)/(internal angle of friction)

SR Average Sediment rate (mm/yr)

L Average Length (in km) between ~2.5-7.5Myr

α Average Taper angle α (in degrees) between ~2.5-7.5Myr

D Average Distance between the first and second frontal thrust between ~2.5-7.5Myr(in km)

T Average time a frontal thrust remains active between ~3.5-7.5Myr

$\langle R_o \% \rangle$ Average vitrinite reflectance of the wedge between ~3.5-7.5 Myr

%_{top} Proportion of >1 eventual $R_o\%$ (*vitrinite reflectance at 7.5 Myr*) at shallow half of the incoming sediment at 2.5 Myr.

%_{bottom} Proportion of >1 eventual $R_o\%$ (*vitrinite reflectance at 7.5 Myr*) at deep half of the concoming sediments.



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Fig. 1: Distribution of thermal maturity for different models at ~7.5 Myr (5 Myr of thermal maturation). Panels A1-A5 show the thermal maturity distribution (computed using Easy%Ro) in subduction wedges of models as a function of décollement strength $M_0^2 - M_0^{22}$, respectively. A6-A10 show the thermal maturity distribution in subduction wedges of models function of sedimentation rate $M_{0.1}^{12} - M_{0.9}^{12}$, respectively. The grey color of the markers indicate that no thermal maturity change in these sediments have not occurred. B1-B10 and C1-C10 similarly show the thermal maturity distribution in subduction wedges computed using Simple%Ro and Basin%Ro-, respectively.

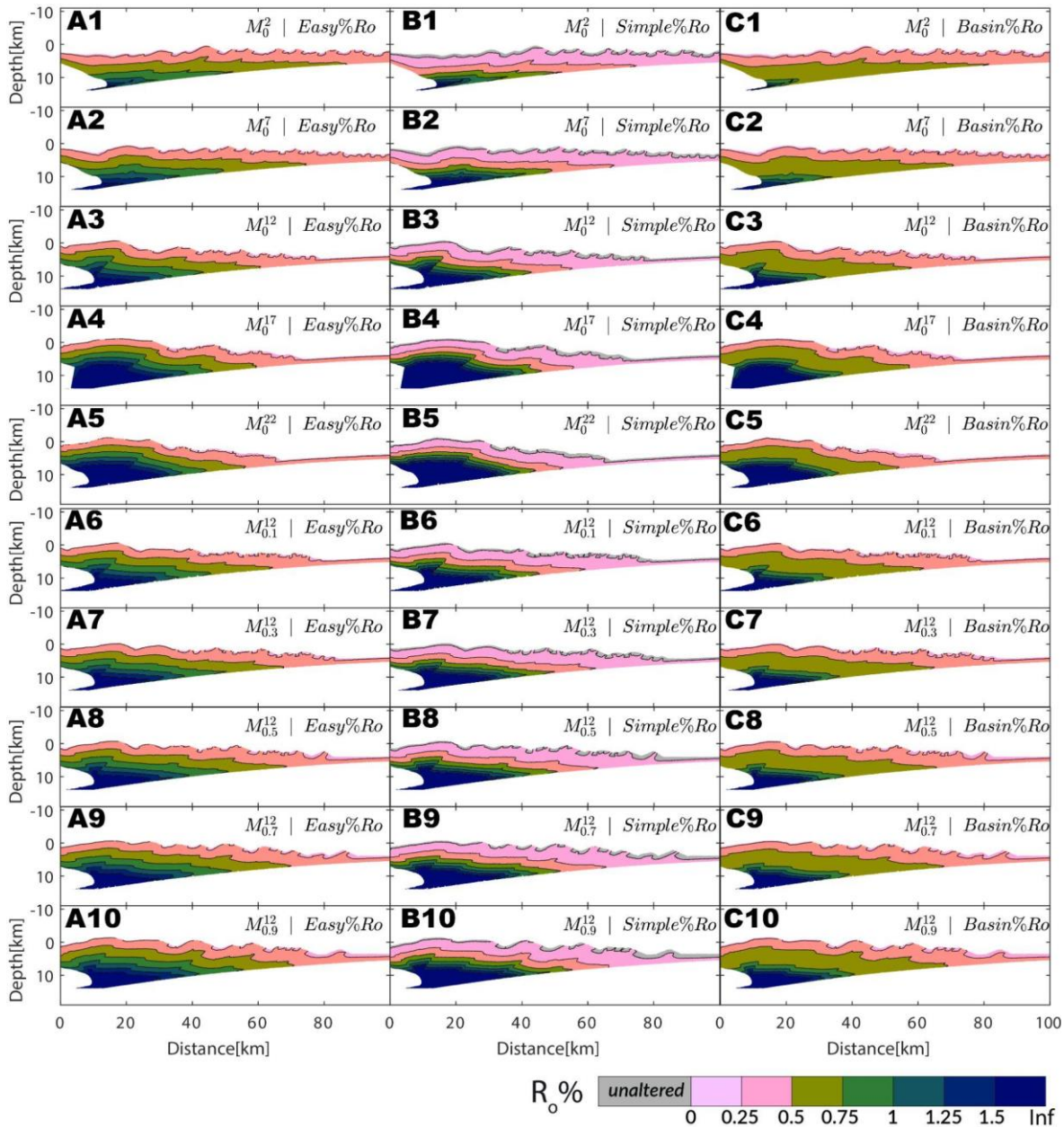




Fig. 2: The variation of % R_0 for an horizon at the trench depth of each model at 7.5 Myr. Panel A shows all the models with different decollement stretch (M_0^2 - M_0^{22}). Panel B shows all the models with different sedimentation rates ($M_{0.1}^{12}$ - $M_{0.9}^{12}$)

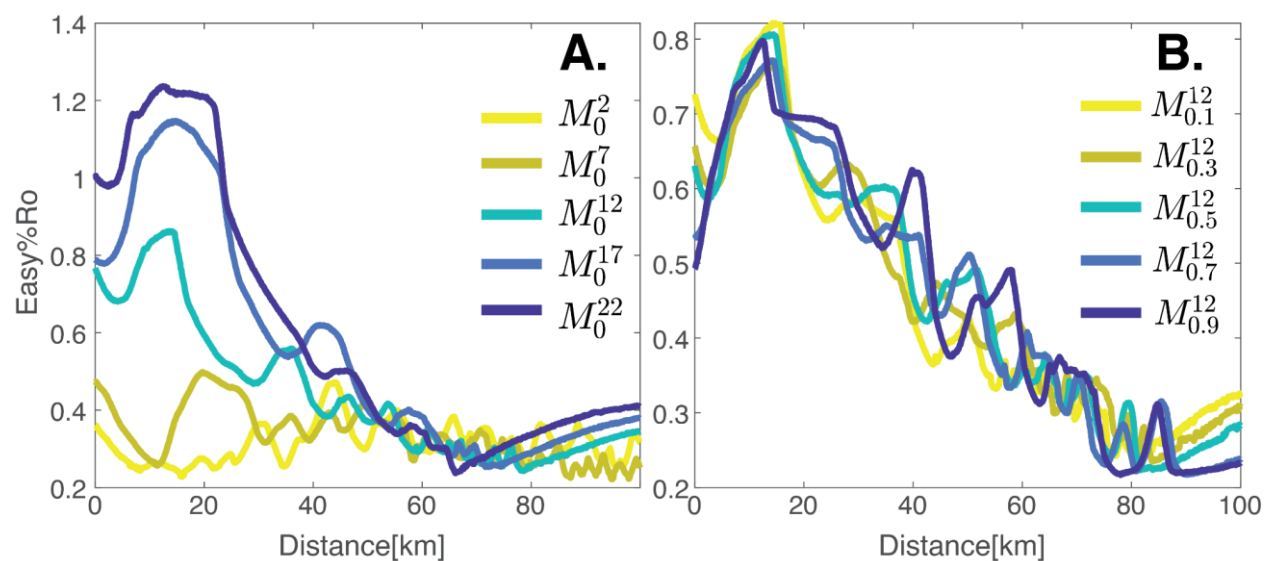
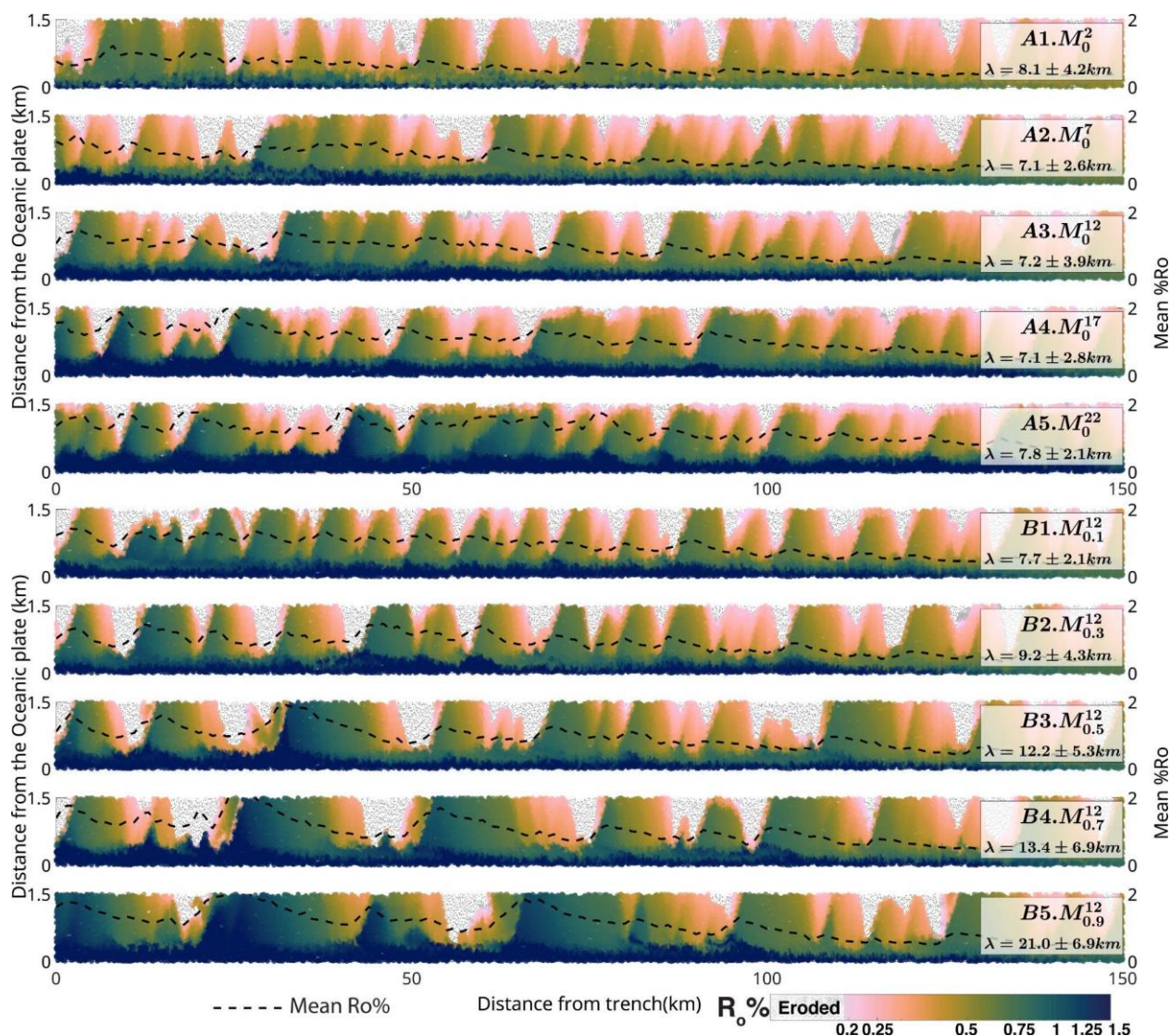




Fig. 3: Map of thermal maturity at 7.5 Myr mapped to sediments at 2.5 Myr. Panel A1-A5,B1-B5 show the mapping for models M_0^2 - M_0^{22} and $M_{0.1}^{12}$ - $M_{0.9}^{12}$ respectively. The vertical axis (distance from the oceanic plate) has been corrected for the bending of the plate. The horizontal axis represents the distance of sediments from the trench. The grey colour of the markers indicates that these sediments have been eroded/reworked due to slope failure. The broken black line represents the mean % R_0 attained sediment at a given distance from the trench. λ represents the horizontal periodicity in mean % R_0 for the given model.



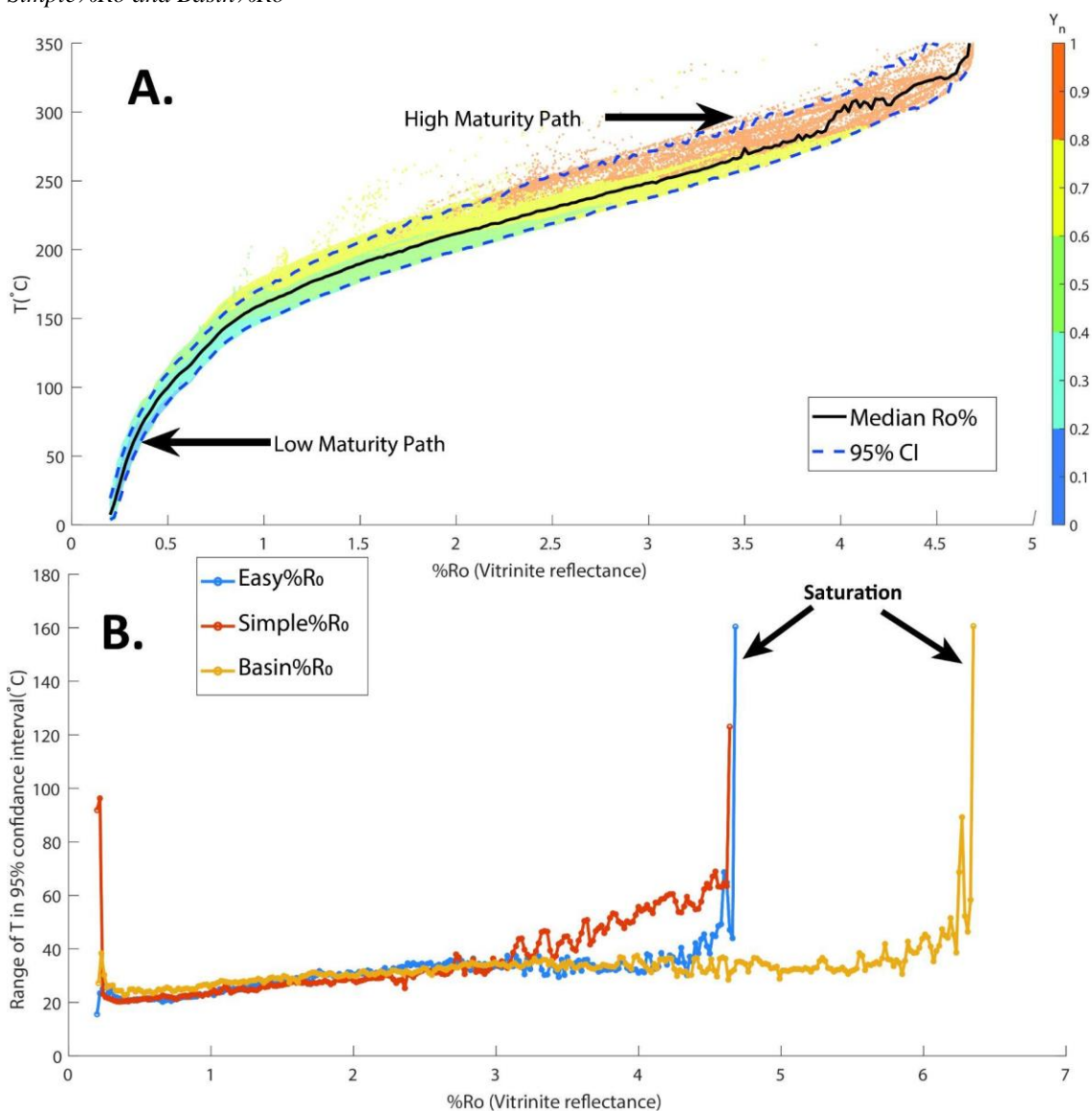




Fig.5: Depth vs Thermal maturity(%Ro). The shaded (in violet) region shows the range of observed $R_o\%$ (mean \pm 1SD) from the C0002 borehole (Fukuchi et al., 2017), colored lines represent the values in models M_0^{12} , $M_{0.1}^{12}$, $M_{0.3}^{12}$, $M_{0.5}^{12}$, $M_{0.7}^{12}$, $M_{0.9}^{12}$.

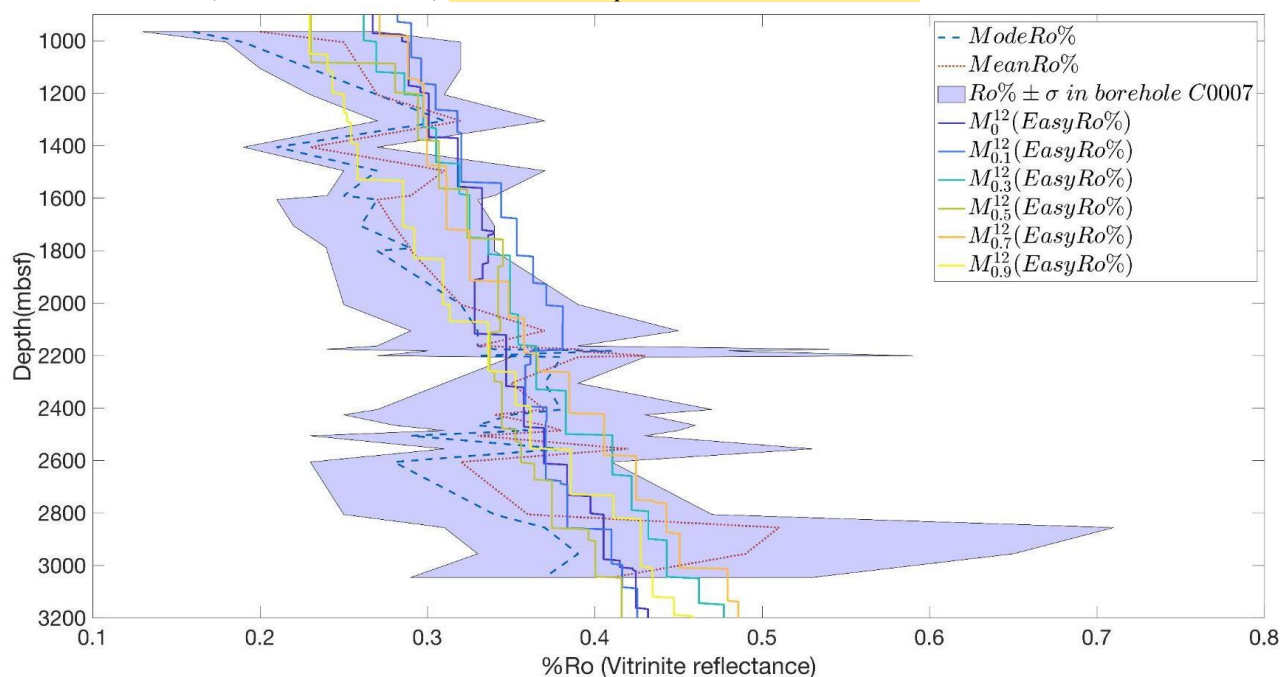




Fig. 6: Panel A Mapping of eventual thermal maturity(vitrinite reflectance at 7.5Myr) to a frontal thrust at ~4Myr in model $M_{0.9}^{12}$. The lithology of the wedge is shown in panel B. The half arrow represents the active frontal thrust.

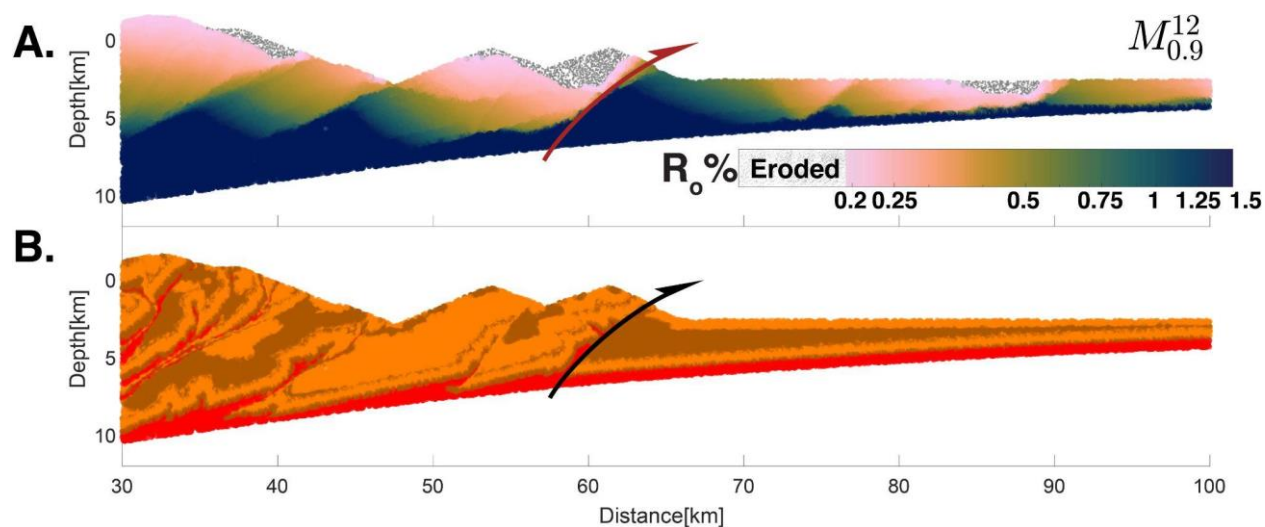




Fig. 7: Position dependency of thermal maturity preservation. **Panel A.** Model state at ~2.5 Myr with a thermal anomaly placed at 110-125 km from backstop **B.** Model state at ~2.5 Myr with a thermal anomaly placed at 140-155 km from the backstop. **C.** Model state at ~7.5 Myr.

