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 underthrusted 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($\%R_0$) using three well-established methods of $\%R_0$ 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

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

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

101   S2).

2.1 An improved thermal maturity calculation

103   Given that assessments of thermal maturity are inherently reliant on the distribution of temperature inside the wedge, any

104   attempt to model thermal maturity needs a realistic temperature gradient in the wedge. We incorporate this by modifying the

105   thermal conductivity computation for sediments and décollement (see Table 1 and section 1 in the provided supplementary

106   text) to match the empirical relationship between depth and thermal conductivity, as measured on core samples in the borehole

107   IODP Site C0002(Sugihara et al., 2014; Tobin et al., 2015). Both for the same accretionary wedge is scarce to find, and to our

108   knowledge, the C0002 borehole in Nankai accretionary wedge along the Kumano forearc basin is the only place with available

109   datasets for both thermal conductivity and thermal maturity values for an accretionary wedge (Fukuchi et al., 2017). The model

110   computes the %R_0 of each marker to estimate the thermal maturity of sediments during the model run using three widely used

111   methods of thermal maturity modelling Easy%R_0 (Burnham & Sweeney, 1989), Simple%R_0(Suzuki et al., 1993) and Basin%R_0

112   (Nielsen et al., 2017). All these approaches for computing %R_0 yield similar trends albeit different absolute values. In the

113   interest of clarity, we have mostly illustrated Easy%R_0, which is the most extensively used method for Vitrinite Reflectance

114   computation. Hence, in the interest of clarity, we have mostly illustrated Easy%R_0, which is the most extensively used method

115   of Vitrinite Reflectance computation. Hence, hereafter we refer Easy%R_0 as simply %R_0, unless explicitly stated. %R_0 is set

116   to 0.2 in sediment markers at the start of the model till 2.5 Myr, while %R_0 in markers for other rocks, air, and water is

117   undefined at all times. After 2.5 Myr, the model computes %R_0 on each marker as a function of temperature (T), time (t), and

118   amount of fixed carbon as a percentage(f_c). The initial %R_0 of newly deposited sediments is computed using an assumed

119   water-sediment interaction temperature assumed to be the same as the thermocline. The thermocline used in the model has

120   been estimated using the data obtained and made freely available by International Argo Program and the national programs

121   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

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125 thermocline. The thermocline used in the model has been estimated using the data obtained and made freely available by

126 International Argo Program and the national programs that contribute to it for the region near Nankai (Fig S3, Argo, 2022).

127 *2.2 Experimental Strategy*

128 Here, we present a total of 10 models that vary in their effective basal friction or their effective sedimentation rate to discern

129 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

130 effective internal angle values for the décollement of ϕ_b= 2°, 7°, 12°,17° and 22° respectively. The chosen range of effective

131 decollement strength is well within the range of values postulated by several studies for the Nankai accretionary wedge(Tesei

132 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

133 variable effective sedimentation rate ranging from 0.1 to 0.9 mm/yr. Sedimentation occurs only at the trench in all of the

134 models presented in this study from sea to land. With these models, we evaluate the particle trajectory and %R_0 of accreting

135 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

136 parameters influencing our observations, models have no erosion. . Moreover, all models lack surface processes during the

137 first ~2.5 Myr and have sedimentation thereafter. Sediments used in the model have an angle of friction of 30° and a strain-

138 softened value of 20° after a threshold of 0.5-1.5 strain. The coefficient of friction increases linearly between the thresholds.

139 Sedimentation rates are the effective sedimentation rate computed after the model run and are thus not prescribed a priori. This

140 choice ensures that the range of average sedimentation in all our models (0.1-0.9 mm/yr) lies within observed sedimentation

141 rates in our chosen natural equivalent, the Nankai accretionary wedge in the south-western subduction margin of Japan(Korup

142 et al., 2014). Table 2 provides more details about the model run and prescribed sedimentary conditions.

143 **3. Results**

144 Subduction begins at 0.1 Myr as the weak material between continental and oceanic plate fails (see supporting information

145 movies). Continued and sustained accretion of sediments against the deforming continental crust forms the accretionary wedge

146 from the interplate contact landwards. After ~5 Myr, all models develop a distinct wedge in agreement with the critical taper

147 theory(Davis et al., 1983). Taper angles increase systematically as effective basal friction increases from ~2° to ~22° (Fig 1,

148 Table 2, $M_0^2 - M_0^{22}$). Whereas models with a relatively weaker décollement, as M_0^2 (ϕ_b= 2°), have taper slopes of 4.3°±

149   0.3°, models with very strong décollement, as M_0^{22} (ϕ_b= 22°), have slopes as steep as 12.8 ± 1.2°(Table 2). Models without

150   trench sedimentation grow solely by accretion of incoming seafloor sediments, with frequent nucleation of frontal thrusts.

151   Models with weaker décollements develop thrusts that are lengthier and remain active for shorter periods. This is clear when

152   comparing, for models with increasingly strong décollement $M_0^2 - M_0^{22}$, the average distance between first and second

153   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

154   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

155   models with similar basal friction, models with higher sedimentation rates have lengthier thrust sheets that remain active for

156   longer periods (Table 2). Steeper surface slopes with increased décollement strengths and change in thrush sheet length with

157   sedimentation and décollement strength are well-known effects that have been confirmed by previous numerical (Mannu et

158   al., 2016; Wang & He, 1999) and analytical(Malavieille & Trullenque, 2009; Storti & Mcclay, 1995) models. All the reported

159   values are mean ± Standard Deviation values recorded between 2.5-7.5 Myr in individual models. All models, exhibit a

160   temperature gradient that corresponds well with the temperature profile observed in the boreholes at IODP Site C0002 in the

161   Kumano forearc basin, on top of the Nankai accretionary wedge (Fig. S4).

162   ### *3.1 Thermal maturity of the wedge*

163   Sediments are more thermally mature in wedges that have a higher sedimentation rate or décollement strength. For example,

164   the mean %R_0 of simulations for wedges with the highest sedimentation ($M_{0.9}^{12}$) is 12% higher (0.75) than in those without

165   sedimentation (M_0^2) (Table 2, Fig 1). Similarly, simulations of wedges with the strongest décollement have the highest mean

166   %R_0 (0.94) of all the simulations presented in this study.

167   Thermal maturity values increase with depth and landward distance from the trench to the forearc high irrespective

168   of the decollement strength, sedimentation rates and method of thermal maturity computation (Fig. 1). As a result, sediments

169   at the core of the wedge consistently reach the highest maturity. The absolute value of %R_0 and the rate at which thermal

170   maturity values increase landward from the trench are larger for wedges with high décollement strength(Fig. 2A). In wedges

171   with the same décollement strength but higher trench sedimentation the rate of thermal maturity increase landward from the

172   trench remain very similar(Fig. 2B). Comparing the values of %R_0 (Fig. 2) along an arbitrary horizon in several models

173   emphasizes this result; the model with the highest décollement strength attains the maximum %R_0 of 1.25, and has the highest

174   rate of landward increase in thermal maturity(Fig. 2A). However, all models with similar décollement strength but different

175   sedimentation do not visibly vary in their rate or magnitude of landward increase in thermal maturity. All models show a

176   decrease in thermal maturity landward of the forearc high, commonly of 0.2 %R_0 . Other interesting observations that we

177   explore below are the increased thermal maturity occurring in the vicinity of thrusts (e.g. Fig 1) and the reversal in sediment

178   maturity around out-of-sequence thrust (e.g. Fig 1) active over longer times visible across several models (Fig 1).

179   The magnitude of %R_0 varies consistently among Easy%R_0, Simple%R_0 and Basin%R_0. On average Easy%R_0 have

180   the smallest values, followed very closely by Basin%R_0(with an average difference of only 0.02). However, Simple%R_0 had

181   the highest average value of thermal maturity being 0.16 and 0.13 higher than Easy%R_0 and Basin%R_0 (Fig 1).

182   *3.2 Sediment trajectory inside the wedge*

183   Sediments follow high-maturity paths in larger proportions in wedges with a higher décollement strength or sedimentation

184   rate. We demonstrate this effect by creating a map of the thermal maturity of sediments at 7.5 Myr of the model run, mapped

185   to their spatial position 5 Myr earlier (at 2.5 My of the model run) (Fig. 3) to analyse the spatial correlation between sediment

186   position (depth and distance) from the trench and thermal maturity. We also show the mean thermal maturity attained by

187   sediments at a given horizontal distance from the trench during this period. The scatter plot shows sharp changes with distance

188   from the trench that relate to changes in sediment trajectory (Fig. 3). The mean thermal maturity is also variable along the

189   horizontal length of the wedge and has a periodicity increasing in distance with higher sedimentation rate but relatively constant

190   with changing basal friction (Fig. 3). Whereas the mean thermal maturity has a short periodicity of ~7.2 km for the model

191   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

192   same no sedimentation M_0^{2}-M_0^{22} the periodicity remains relatively consistent between the range of 7-8 km.

193   Fig 3 also represents the distribution of trajectories that exist in an accretionary wedge and how these trajectories get

194   impacted under trench sedimentation(a subset of these trajectories can be viewed in the supplementary Fig. S5). Whereas in

195   wedges with weak decollements (M_0^{2}), none of the shallowest half of incoming sediments reach %R_0 > 1 in 5 Myr, 2% of

196   sediments reach this value in wedges with strong décollement (M_0^{22}). The effects of décollement strength in the thermal

197   maturity of sediments can be quantified as well at deeper levels, with one-eighth vs more than half of the sediments surpassing

198   values of %R_0 = 1 for the deepest half of incoming sediments (12.0% and 54% respectively) in weak vs strong-decollement

199   wedges(M_0^2 vsM_0^{22}), respectively. Increasing the sedimentation rate shows this effect even more prominently. In wedges

200   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

201   %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

202   bottom half of the wedge that reach high maturity steadily increases with both sedimentation rate and décollement strength

203   (Table 2).

204   *3.3 Patterns of trajectory and thermal maturity in incoming sediments*

205   The diversity in the trajectory of sediments in the wedge leads to a plethora of pathways in which the sediments can become

206   thermally mature and thus introduces epistemic uncertainty in the estimation of maximum exposure temperature. Fig 4,

207   captures this uncertainty where we plot the maximum exposure temperature as a function of %R_0 for all the models simulated

208   in this study. We find that almost all the models show a remarkable similarity in their relationship between maximum exposure

209   temperature and %R_0 (for individual models please see Fig S6) and differ mostly in their proportion of sediments with extreme

210   values of %R_0. We observe that the typical uncertainty in maximum exposure temperature increases with an increase in values

211   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,

212   Fig. 4b). Furthermore, we observe that information about the present depth of the sediments w.r.t the thickness of the wedge

213   (as represented by different colours in Fig 4a) greatly helps to further constrain the maximum exposure temperature. For

214   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

215   greatly reduces to only ~10.5°C. Thus the range of thermal maturity values for sediments clearly has a large correlation with

216   their trajectories.

3.4 Comparision 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 %R_0 (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 %R_0 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.,

290   2016, 2017; Mugnier et al., 1997; Simpson, 2010; Storti & Mcclay, 1995), and the effect of each of these factors can be

291   accounted for when assessing the trajectory of sediments and the distribution of thermal maturity in accretionary wedges.

292   Sediment mixing in subduction wedges is primarily controlled by thrusting. Previous studies have reached seemingly

293   contradicting outcomes when using numerical(Miyakawa et al., 2019; Wenk & Huhn, 2013; S. Willett et al., 1993) and

294   analogue(E. Konstantinovskaia, 2005; Mulugeta & Koyi, 1992) approaches to analyze sediment trajectories as a function of

295   changes in erosion, sedimentation, or décollement strength. While some studies showed that the rate and extent of a transition

296   by which sediment trajectories change from generally horizontal to increasingly vertical during accretion change consistently

297   with the initial depth of incoming sediments(Mulugeta & Koyi, 1992; S. Willett, 1992), others predicted different crossover

298   paths for sediments accreting over a range of décollement strengths(E. Konstantinovskaia, 2005). Our models show that both

299   are valid results and that changes in trajectory patterns leading to path crossovers are controlled by the horizontal distance of

300   sediments from the frontal thrust. Starting at a threshold distance from the trench, sediments at different depths follow laminar

301   paths along different trajectories within the wedge. Laminar-type trajectories can be reproduced in a broad range of simulations

302   and are particularly common in models with low sedimentation and décollement strengths. However, the depth dependence of

303   sedimentary paths varies periodically as a function of distance from the trench of specific sedimentary packages (Fig. 3,6).

304   This effect, which is particularly marked in the neighbourhood of the frontal thrust, explains the crossover paths for incoming

305   sedimentary packages at similar depths and different horizontal locations, as shown by Konstantinovskaia et al. 2005.

306   Therefore, thrust faults in the wedge act as the primary agent controlling whether sediments sustain depth-controlled laminar

307   flow or mix.

308   The thermal maturity that incoming sediments reach varies periodically as a function of thrust frequency. Although

309   previous research considered non-laminar sediment trajectories as chaotic(Mary et al., 2013), and the wide variety of

310   trajectories shown in our models seem to agree with this (Fig 3, Fig S4), patterns emerge when we correlate the lateral and

311   vertical position of incoming sediments with their eventual thermal maturity. Changes in the depth of the thermal maturity

312   boundary are less frequent and have larger amplitudes with increased décollement strength, and especially, increased

313   sedimentation rates (Fig. 4). The periodicity in the thermal maturity boundary marks the periodic oscillation of the predominant

314   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 $\%R_0$ 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

overthrusted 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

affect only sediments at the deeper locations of the sedimentary pile, which are in turn the sediments that most likely to follow

a high-maturity path. We thus regard the possibility of retrieving such antecedent geothermal information as minimal.

The main implications of this contribution emerge from its predictive power. Our approach can predict to a precise the thermal

maturity of sediments and the uncertainty associated with the maximum exposure temperature in accretionary contexts with

known structuration. More accurate quantification of the thermal evolution and thermal state of accreted sediments reduces

the uncertainties attached to the location of temperature-led transformations of organic material into hydrocarbons in

subduction margins and other accretionary contexts. Such increased accuracy in the distribution of thermally mature sediments

may also be applied for improved assessments of the evolution in time of any other geothermal process, including seismic slip,

magmatic and metamorphic extent, porosity, compaction and diagenesis of sediments, and the reconstruction of convergent

margins in general(Bostick & Pawlewicz, 1984; Ferreiro Mählmann & Le Bayon, 2016; Rabinowitz et al., 2020; A. Sakaguchi

et al., 2011; Totten & Blatt, 1993; Underwood et al., 1992).

Finally, among the three methods of $\%R_0$ computation, Easy$\%R_0$ and Basin$\%R_0$ are clearly more consistent and well-

constrained on a wide range of thermal maturity in comparison to Simple$\%R_0$, which seems to be particularly useful for a

smaller range of thermal maturity values. This simply illustrates the fact that while Easy$\%R_0$ and Basin$\%R_0$ computation

deals with several parallel reactions related to the maturity of kerogen(and hence multiple activation energies), the Simple$\%R_0$

is based on best-fitted single activation energy, and hence yields large confidence intervals at the extreme $\%R_0$ values.

Additionally, the inclusion of the higher activation energy reactions in Basin$\%R_0$ makes it the best-suited formulation for

sediments at the deeper and shear zone sediments which usually get saturated using Easy$\%R_0$.

4. Conclusion

This study demonstrates how contractional faults alter the paths of sediments as they accrete and how this fundamentally

controls the distribution of the thermal maturity of sediments in accretionary wedges and emphasizes the role that

sedimentation rate and interplate contact strength have in such distribution. The increased resolution of our approach leads to

findings that have relevant implications. For example, the geothermal history that can be retrieved from the thermal maturity

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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507   **List of Tables**

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

Rock Type	Density (kg/m³)	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(-Z²/1.3e7))	Wet quartzite	154	2.3
Sediments1	2600	0.5/0.05*	4.64/0.2*	(0.96+807/(T+77))* (1-exp(-Z²/1.3e7))	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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511 *Table 2: Model runs and their specific characteristic observations*

Models	φ_b	φ / φ_{ss}	SR	L	α	D	<R_o%>	%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
<R_o%> 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. 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 strench (M_0^2-M_0^{22}). Panel B shows all the models with different sedimentation rates ($M_{0.1}^{12}$-$M_{0.9}^{12}$)*
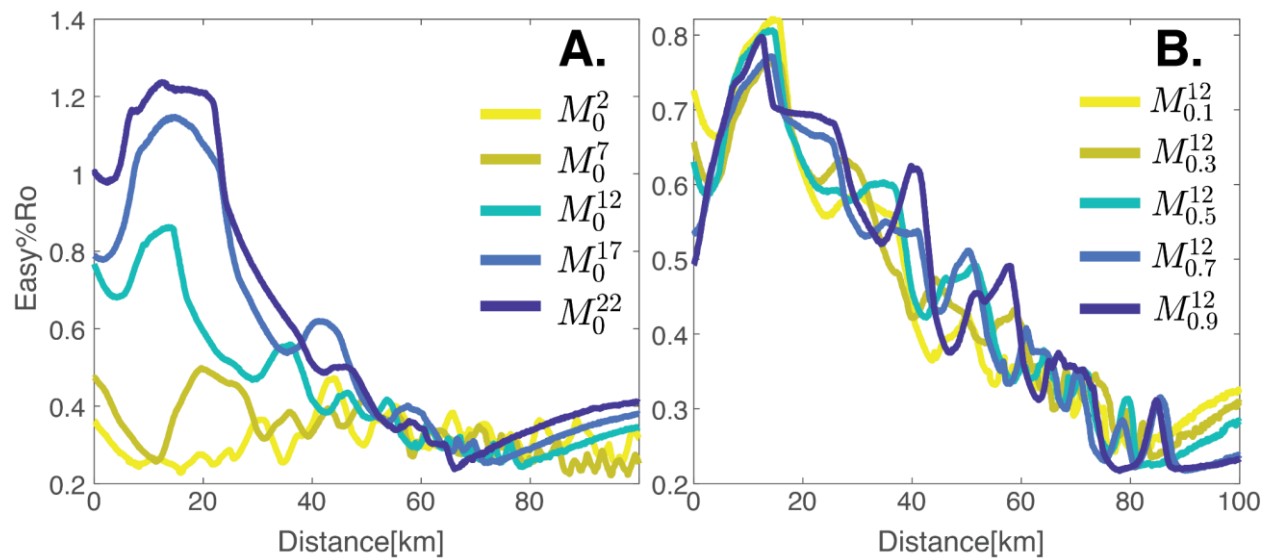
Fig. 3: *Map of thermal maturity at 7.5 Myr mapped to sediments at 2.5 Myr. Panel A1-A5,B1-B5 show the mapping for models M_0^2-M_0^{22} and $M_{0.1}^{12}$-$M_{0.9}^{12}$ respectively. The vertical axis (distance from the oceanic plate) has been corrected for the bending of the plate. The horizontal 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.*

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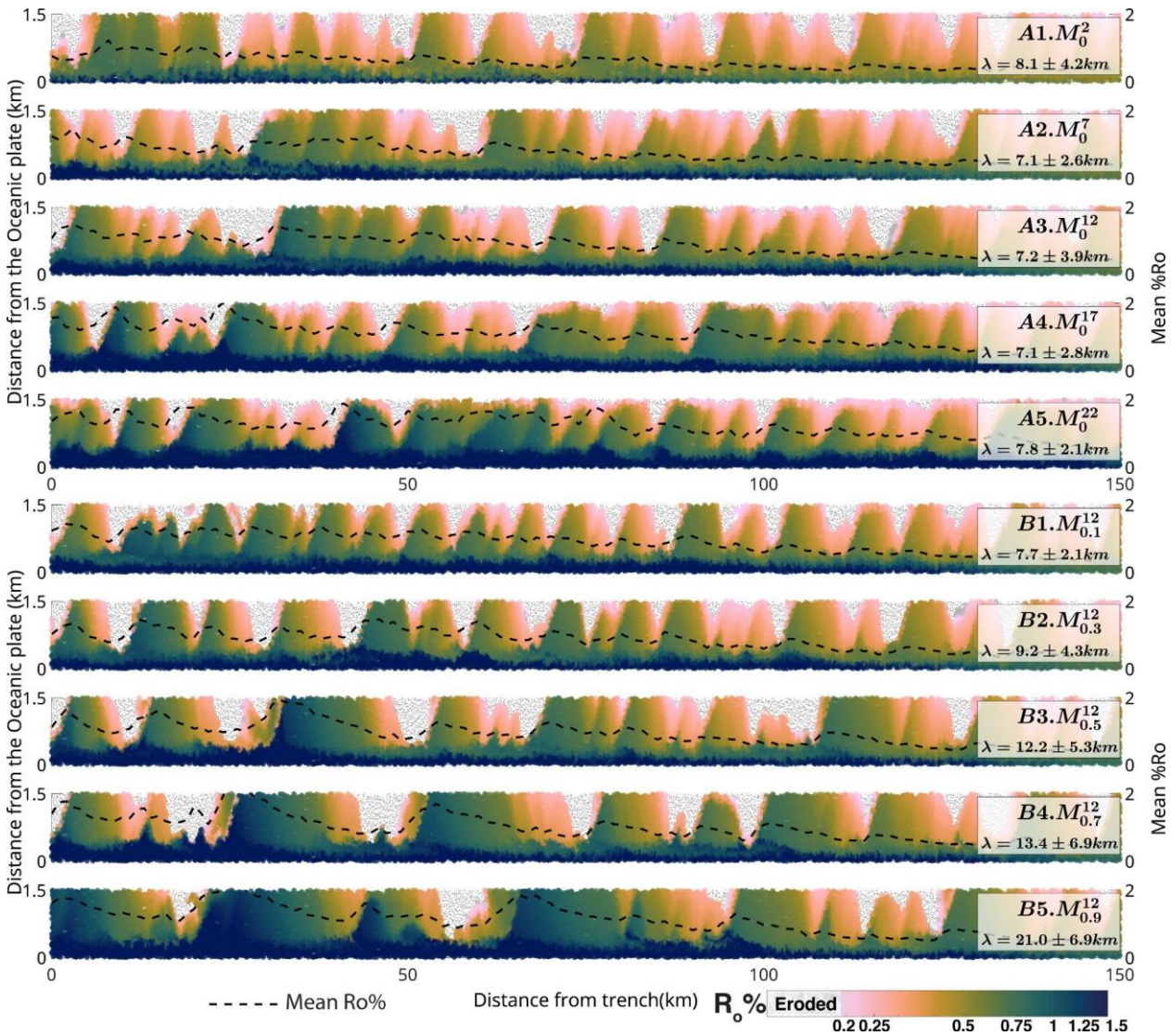
534 *Fig: 4 A. Vitrinite Reflectance(R_0%) vs Maximum Exposure temperature in all models **B.** Range of 95% CI for Easy%Ro,*

535 *Simple%Ro and Basin%Ro*

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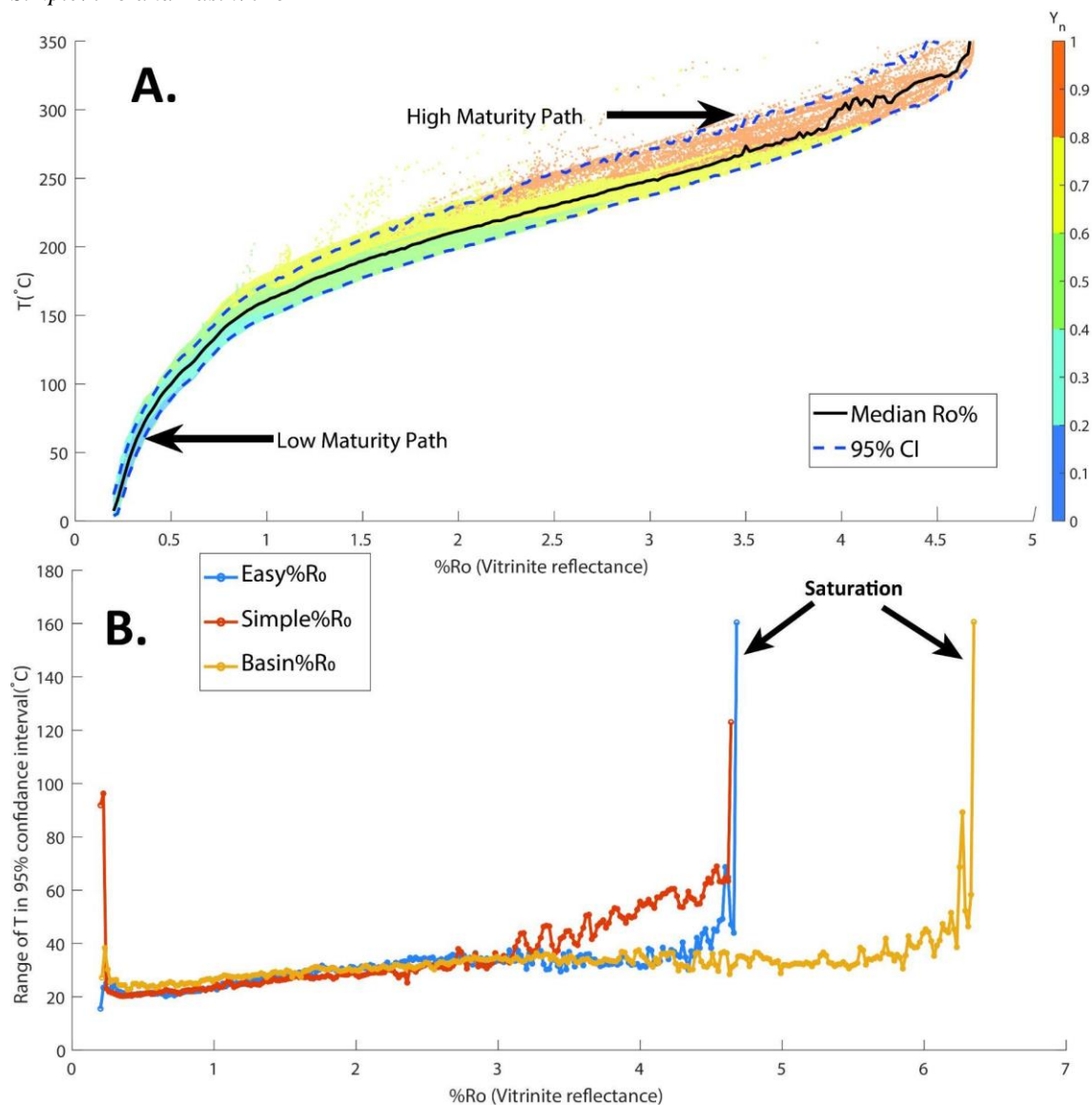
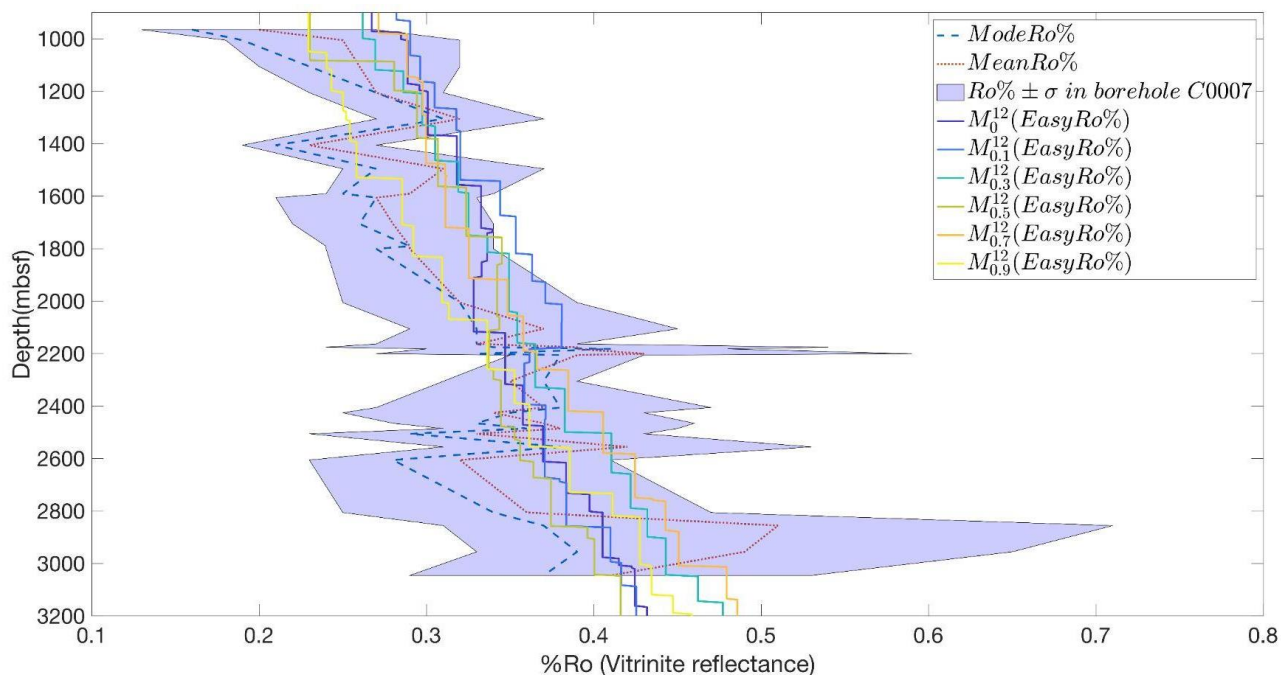


Fig.5: *Depth vs Thermal maturity(%R$_0$). The shaded (in voilet) region shows the range of observed R$_o$%(mean±1SD) from the C0002 borehole (Fukuchi et al., 2017),colored lines represent the values in models* M_0^{12}, $M_{0.1}^{12}$, $M_{0.3}^{12}$, $M_{0.5}^{12}$, $M_{0.7}^{12}$, $M_{0.9}^{12}$.

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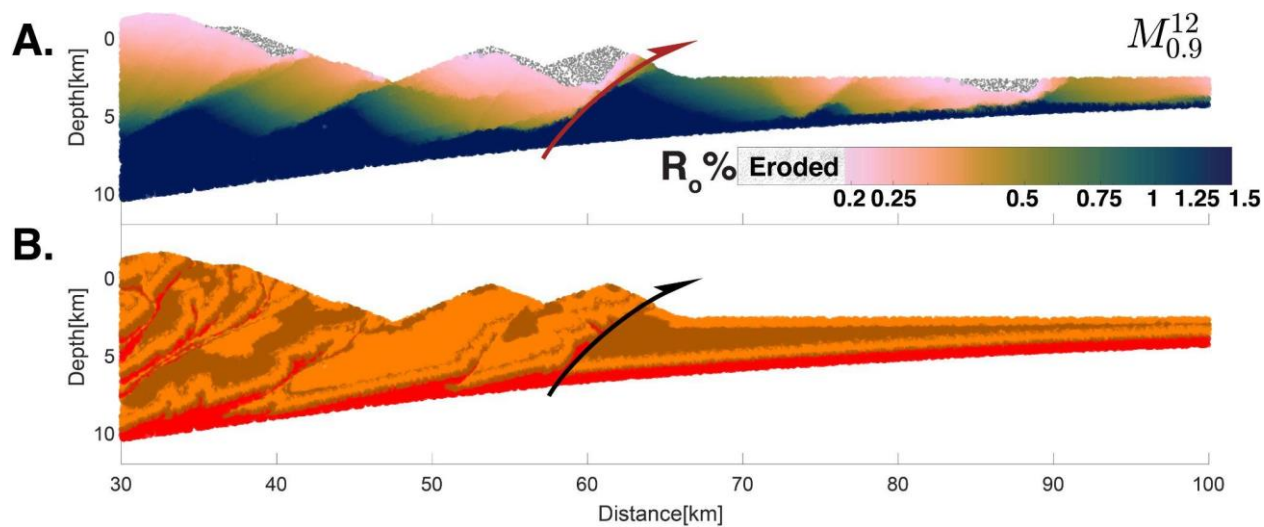
566 **Fig. 6:** *Panel A Mapping of eventual thermal maturity(vitrinite reflectance at 7.5Myr) to a frontal thrust at ~4Myr in model*
567 $M_{0.9}^{12}$. *The lithology of the wedge is shown in panel B. The half arrow represents the active frontal thrust.*

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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.*