Note S1, Description and interpretation of sedimentary facies and its evolution

Xianghui Li[1], Jingyu Wang[1], Troy Rasbury[2], Min Zhou[1], Zhen Wei[1], Chaokai Zhang[1]

[1]State Key Laboratory for Mineral Deposits Research, School of Earth Sciences and Engineering, Nanjing University, Nanjing 210023 China. Email: leeschhui@126.com

[2]Department of Geosciences, Stony Brook University, Stony Brook, NY 11794-2100, USA

1. Observation and description of sedimentary facies

Field observation and description were executed on six outcrop sections (Locations A1 to A4, A6 and A7, Fig. 1). Much attention has been given to lithologies, textures, sedimentary structures, stratal occurrences, and faunal contents during the field observation. Aquatic invertebrate fossils and carbonates have been particularly applied to help interpret the lake environment. Lithofacies interpretation relies on the published description from references for those unobserved sections (Locations A5, A8, and A9, Fig. 1).

Microscopic examination of sedimentary rocks further aided in the interpretation the depositional conditions for environments. Grain size, sorting, roundness, and matrix type and content are carefully checked and described to determine both texture and component maturity. About forty lithological samples were collected and twenty ones were polished thin-sections from the six cross-sections (Figs. S1 and S2).

2. Lithofacies classification

Based on the investigation of cross-sections (locations A1-A4, and A6-A7 in Fig. 1), terrestrial depositional environment units, such as alluvial fan, fluvial river, flood plain, lake, lake-delta, swamp, were detected with corresponding lithologies of the continental Lower Jurassic sequence in the grand Sichuan paleobasin (GSB).

2.1. Alluvial fan facies

Alluvial fan facies are characterized by coarse terrigenous clastics. Blocky medium-coarse conglomerates are the dominant lithology, in which gravels are mainly quartz arenites, and a few limestones as well as other rocks. Gravels (pebble, cobble, and boulder) are moderate-well round and sorting with indistinct sieving and imbricating structures (Fig. S3a). Conglomerates often occur as lenticular beds. This lithofacies developed in the basal and lower Baitianba Fm in northern and western margins of the basin (e.g., Gou, 2001; He et al., 2013; Qian et al., 2016; and this work. Fig. 1).

2.2. Fluvial facies

The fluvial facies is composed of medium-thickness lithic sandstones (Fig. S4a) associated with siltstones and mudrocks. A variety of tractive sedimentary structures can be found in the sedimentary sequence. And subfacies, such as channels (Fig. S3b and S3c), inter-channels, point-bars (river island), levees, and overbanks, are readily recognised. The facies is particularly distinct and abundant in Ya'an region, southwestern GSB (Fig. S1). Though this facies was marked in large area of the eastern GSB margin (western Hubei-Hunan), no lithofacies sections were provided and studied (figure 6 in Li and He, 2014).

2.3. Flood plain facies

Flood plain facies are composed of reddish-brownish mudrocks and siltstones, of which the former is relatively thick and the latter is thin stratification (Fig. S3d). Sometimes this facies is associated with drained fluvial riverine facies, leading to difficult differentiation with the overbank subfacies in the river system. This is because both are dominated by fine sediments with some fossils of plants and aquatic invertebrates and ripples. This facies is particularly common in the central basin (Figs. 1, 2, and S1), and also distributed in western and northern margins of the GSB (Fig. 1).

2.4. Lacustrine facies

Lacustrine facies is widespread through the lower Jurassic Ziliujing Fm in the whole GSB (Figs.1, 2, and S1). The typical lacustrine facies is composed of carbonates (Fig. S3e and S3f), sometimes associated with medium-fine terrigenous rocks. Carbonates, such as laminated dolomitic mudrocks (Fig. S4b), argillaceous micritic dolomites (Fig. S4d), and coquina (Figs. S4e-S4f), are readily observed in both field (Figs. S3e-S3f) and under microscope (Fig. S4). Burrows are abundant in this facies (Fig. S1).

Lacustrine lithofacies can be subdivided into shore/littoral, shallow, and deeper subfacies. The lakeshore subfacies is characterised by fine quartz arenites (Fig. S4c), siltstones, and / or dolomitic mudstones or limy dolomites as well as bioclastic grainstone (Fig. S4f). Shallow lake subfacies is composed of mudstones, coquina, mudrocks, and siltstones, of which separated shells of bivalves (Fig. S4e), conchostracans, and ostracods are well preserved without abrasion. Deeper lake subfacies consists of darker shales interbedded/intercalated with thin-bedded mudstones and wackstones (e.g., Bed H6 and H11 in Tanba section, Hechuan. Fig. S2).

Limy breccia can be observed in the Ziliujing Fm when lacustrine limestones are relatively thick (> ~5 m). Breccias often accompany with karstificated caves (Fig. S5). Karst breccias occur in the Dongyuemiao Fm at the Shaping section, Ya'an (Figs. S1, S5a and S5b) and in the upper Da'anzhai Fm at the Tanba section, Hechuan (Figs. S2, S5c and S5d).

2.5. Delta facies

Greyish medium-fine lithic sandstones and shales mainly comprise the lacustrine delta facies. Sedimentary structures, such as trough cross-bedding, parallel bedding, ripple, and wave-mark are well documented in sections of northern Sichuan Basin (Locations A1 to A3 in Fig. 1. Delta facies interpretation shown in Fig. S6). Due to lack of subaerial records, the greyish hue, sedimentary structures, and lithologies indicate a dominant deltaic front subfacies, in which subordinate subfacies of distributary channel, distal estuarine sandy-bar, interbar and interchannel can be differentiated. However, this facies as a whole chiefly occurs in northern and northwestern margins of the GSB (Figs. 1 and S6).

2.6. Palustrine facies

Wetlands have been considered to be (partly) lacustrine environments (Armenteros et al., 1997). Palustrine facies has been viewed as a component of the lacustrine-palustrine facies system and has been applied as a subcategory of the lake environment, especially in pre-Quaternary sedimentology (e.g., Platt, 1989; Platt and Wright, 1992). Here we interpret palustrine facies as an independent and approximate lithofacies, which corresponds to the marginal lacustrine subfacies (Platt, 1989) or interchannel.

The palustrine facies is distinct with thin coal layers and coal seams in the observed sections. The plant fossils in the coal layers are dominated by low diversity ferns (summary refers to Wang et al, 2010). This lithofacies is often associated with the lakeshore subfacies, and mostly occurs in the lowest Lower Jurassic, i.e. in the Qijiang Member (Fig. S2) and the lower Baitianba Fm (Fig. S6).

3. Sedimentary evolution

Together with the Yunnan basin, the GSB had switched to the terrestrial environment from the continental epiric sea since the Late Triassic Indosinian orogeny in Southeast and East Asia, and it had been dominated by drainage river system during the Norian and Rhaetian of the Late Triassic (e.g., Liu and Xu, 1994; Ma et al., 2009). Thereafter, both of the GSB and grand Sichuan paleolake (GSL) were greatly increased in size (~ 480,000 km^2 and 380,000 km^2, respectively. Fig. 1) and the GSB had become a lake-dominant environment (e.g., Ma et al., 2009; Li and He, 2014). Correspondingly, sedimentary lithofacies had been temporally changed in the GSB.

At the beginning of the Early Jurassic, limited sediments of two lithostratigraphic units are documented. The main stratal representative is the Qijiang Mem, which had been deposited in lakeshore and swamp environments (Fig. 7) and only occurs in part of the southern and central GSB (Locations A6, A7, and A8. Figs. 1 and 6). The other one is the Baitianba Fm, and coarse clastic and coal-bearing rocks in its lower part only corresponds to the earliest Jurassic sediments (Fig. S6), which were deposited in alluvial fan-plain and swamp (He et al., 2013; Qian et al., 2016; and this work) in the northern margin of the GSB (Fig. 1). The local distribution of the two units indicates that the depositional extent was relatively small in the GSB, and implies a hiatus between the Upper Triassic Xujiahe Fm and Lower Jurassic Ziliujing Fm and/or Baitianba Fm (Table 1 and Fig. 7) as a paraconformity suggested by SBGM (1991, 1997).

Above the Qijiang Mem is the Zhenzhuchong Mem, mainly deposited with medium-fine terrigenous clastic sediments. This member is largely distributed in the GSB with different lithofacies. Riverine and flood plain lithofacies are dominant in west (sections A4 and A5. Wen and Zhao, 2010; Wang et al., 2006; and this work), east (section A7. Wang et al., 2006), and south (sections A8 and A9. Zhang et al., 2016; Li and Chen, 2010) of the GSB, and flood fan facies is associated with lakeshore sublithofacies (section 6) in the center of the grand basin (comp sections in figure 7). It was predominated by the lacustrine delta facies in the northern margin of the basin although an exact correlation (possibly the middle Baitianba Fm) is difficult in age (Fig. S6). From the lithofacies and sedimentary distribution, the Zhenzhuchong Mem could represent the record of the largest extending basin, i.e. the final formation of the GSB.

The Dongyuemiao Mem is mainly composed of limestones with or without intercalations and/or interbeddings of (shelly) siltstones and mudrocks. Aquatic shelly fossils and limestones (mudstone, wackstone, and coquina) indicate a shallow lake environment. The lacustrine facies is widespread in the GSB even if this member is thin (~ 8-50 m). It can be recognized through all the observed and correlated sections (Fig. 7), but cannot be exactly correlated to those sections in northern margin of the GSB (Fig. S6). The shallow lacustrine Dongyuemiao Mem outcrops from west (Location A4. Wen and Zhao, 2010; and this work) to east (Location A5. Wang et al., 2006) and from south (Locations A8 and A9. Zhang et al., 2016; Li and Chen, 2010) to center (Location A5 and A6. Wang et al., 2006; Wang et al., 2010; and this work), and the shallow-deeper lake counterpart was diagnosed from both outcrop and drills in north (Fig. 1. e.g., Ma et al., 2009; Ding et al., 2013; Li and He, 2014). Obviously, the occurrence of the lacustrine Dongyuemiao Mem demonstrates the first lake transgression in large scale, probably extending to ~80-90% area of the GSB (Figs 1 and 6), in the Early Jurassic.

Upwards, the Dongyuemiao Mem is sequentially replaced by the siliciclastic Ma'anshan Mem. Mudrocks, siltstones, and sandstones comprise the Ma'anshan Mem, and the rock ratio differs in different location of the GSB. In western and southern margins (Locations A4 and A8. Wen and Zhao, 2010; and this work), the ratio of sandstone + siltstone vs. mudrock is about 1:1-2, but in central and eastern margins (Locations A5-A7. Wang et al., 2006; Wang et al., 2010; and this work) this ratio highly decreases to 1:5-10 (Fig. 7). Based on sedimentary structures and lithological associations, this member is interpreted to have been mainly deposited in river and flood plain in the surrounding margins (e.g. Locations A4-A5, A7-A9) and in flood plain and lakeshore in the central basin (Location A6), indicating that the GSL had been northward regressed at the time.

The Da'anzhai Mem has received attention due to important shale-oil exploration. Besides of the observed and compared sections in figure 6, both of outcrops and geophysical logs have been previously investigated in the northern and central GSB, where deeper lacustrine facies occur (Fig. 1). The Da'anzhai Mem contains mixed carbonates and mudrocks with a few siltstones (Fig. 7). Limestone (mudstone, wackstone, and coquina) and micritic dolomites with shelly fossils indicate the lakeshore and shallow lacustrine subfacies in most areas of the basin (Fig. 7). Shelly carbonate beach subfacies and deeper lacustrine shale-mudstone subfacies are observed in the central and northern GSB, such as areas between Hechuan and Nanchong (Zhu et al., 2013; Shi et al., 2015), Huilong of southern Mianyang (Tan et al., 2016), Yuanba of Guangyuan (Zhou and Liang, 2017), Longgang of northern Nanchong (Ding et al., 2013). The lacustrine facies of the Da'anzhai Mem can be seen across the GSB, not only in margins of west (Locations A4 and A5), east (Location A7), and south (Locations A8 and A9), but also in northern margin (Locations A1-A3 in Figs. 1 and S6) and centre (Locations A5-A6 and other places, Ding et al., 2013; Zhu et al., 2013; Shi et al., 2015; Tan et al., 2016; Zhou and Liang, 2017). This lacustrine facies occurrence indicates a large lake was widespread in the GSB (Fig. 1), implying the second lacustrine transgression happened during the deposition of the Da'anzhai Mem.

In summary, there are two lithofacies sequences/cycles in the Lower Jurassic Ziliujing Fm. The first is the riverine and flood plain lithofacies of the Qijiang Mem and Zhenzhuchong Mem succeeded to the lacustrine facies of the Dongyuemiao Mem, and the second is the flood plain and river facies with swamp lithofacies of the Ma'anshan Mem proceeded to the lacustrine facies of the Da'anzhai Mem. In simple words, twice large lacustrine transgressions had ever taken place in the Early Jurassic in the GSB, Southwest China.

Further carbon and oxygen isotope works of lacustrine carbonates indicate that the GSL had been in a relatively closed hydrological condition. As we know, the covariance proxy of the stable isotopes is a feasible selective for paleoenvironmental interpretation. The covariance of $\delta^{13}C$ and $\delta^{18}O$ values has been used to distinguish between carbonates precipitated in closed or open lakes (e.g., Talbot, 1990; Li and Ku, 1997). Generally, closed lakes have their own positive covariant trends, hydrologically open lakes have little covariance and a limited range of $\delta^{18}O$ values (e.g., Talbot, 1990; Valero Garcés et al., 1997; Alonso-Zarza and Calvo, 2000), and a direct coupling $\delta^{13}C$ and $\delta^{18}O$ is normally considered typical of evaporitic systems (Talbot, 1990; Talbot and Kelts, 1990). We applied this criterion for paleoenvironmental analysis to the late Early Jurassic lacustrine facies in the GSB.

Binomial functions and covariance ratios between $\delta^{13}C$ and $\delta^{18}O$ values are obtained by regression for the carbonate lacustrine facies (Fig. 5). The covariance between carbon and oxygen isotope values shows particularly positive for the carbonate from Shaping section, Ya'an (Location A4, this work), and displays moderate covariance from both Gongjing, Zigong (Location A5, Wang et al., 2006) and

Tanba, Hechuan (Location 6, Wang et al., 2006). The fact that the covariance ratio is very high ($R^2 = 0.957$, $R > 0.978$) and linear for the carbonates from the Shaping section indicates a closed lake system in the western margin of the GSL. The covariance ratio is a somewhat high ($R^2 = 0.467$-437, $R > 0.683$-661) and binomial for the carbonates from sections of Zigong and Hechuan likely signifying a semi-closed lake system in the central GSL. A relatively high ($R^2 = 0.568$, $R > 0.754$) covariance ratio was obtained between the three locations, indicating the relatively closed lake system of the GSL (Fig. 5).

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