Modelling the atmospheric transport distance of PAHs at remote cold regions

CHONGYING LI¹², MEIHAN LI³ AND CHAOQI YU¹

¹ College of Materials and Chemistry & Chemical Engineering Chengdu University of Technology, Chengdu 610059, China, lichy@cdut.edu.cn

² Mineral Resources Chemistry Key Laboratory of Sichuan

³ College of Foreign languages and Cultures, Chengdu University of Technology, Chengdu 610059, China, 317292496@qq.com

Long-range atmospheric transport (LRT) of polycyclic aromatic hydrocarbons (PAHs) means the contamination of remote regions such as high mountains. A simple model was developed to estimate the atmospheric transport distance of PAHs at high mountains, especially lighter PAHs like anthracene and phenanthrene.

This model was made by using the OH reaction rate constant difference between PAH isomers(anthracene and phenanthrene) based on considering isomers gas/particle partitioning, reaction with OH radicals, dry and wet deposition, air-surface exchange and dilution of atmospheric dispersion along transport path in atmosphere as follows.

$$D_{t}(km) = -\frac{6 \times 10^{6}}{C_{OH}(molecules \cdot cm^{-3})} \times windspeed(ms^{-1}) \times \ln \left(\frac{C_{st}^{A}}{C_{st}^{P}} \times \frac{C_{g0}^{P}}{C_{g0}^{A}}\right)$$

Where D_t (km) is the transport distance C_{OH} is the atmospheric [OH]. windspeed is the wind speed of the PAH-containing air masses. C_{g0}^P/C_{g0}^A is the diagnostic ratio(PHEN/ANTH) of anthracene and phenanthrene at emission source , and C_{st}^A/C_{st}^P is the diagnostic ratio (ANTH/PHEN) of anthracene and phenanthrene in snow at sampling location of cold regions.

The model can be used to predict the maximum transport distance and delineate a border of potential emission regions of PAHs at remote sampling sites. The model gave the origin of PAHs in snow at the typically sampling sites in cold regions in Europe and China under a wind speed of 60 m s⁻¹ and 24 h atmospheric average [OH] of 0.3x10⁶ molecules cm⁻³ based on some published data. It is concluded that PAHs at the three sampling sites in Europe primarily came from Europe and Northern Africa at a distance of less than 3000Km and PAHs at the two sampling sites in China came from local regions at a distance of less than 1000Km which are similar to the reports in the literatures.

This work was supported by the National Natural Science Foundation of China (41073085) and Construction plan of research innovation team of Sichuan province universities (12TD001).

The marine biogeochemical carbon cycle modeling of Yangtze sea during the Ediacaran–Cambrian transition

Da Li^{1*}

¹State Key Laboratory for Mineral Deposits Research, Department of Earth Sciences, Nanjing University, Nanjing 210093, China (* lida@nju.edu.cn)

Earth's biosphere witnessed a revolutionary change from soft bodied animals to skeletal animals across the Ediacaran–Cambrian boundary and is associated with frequent large oceanic $\delta^{13}C$ oscillations. The $\delta^{13}C$ excursions are often interpreted to reflect changes in the global carbon cycle. We have reported a 300m-thick high-resolution carbonate $\delta^{13}C$ profile for the Ediacaran–Cambrian Xiaotan section, South China, showing a large negative excursion (N1, -12.2%) in terminal Ediacaran and a sustained pre-'Tommotian' positive plateau (P4, up to +7.3%) which coincides with the occurrence of the Watsonella crosbyi Assemblage SSF [1].

Here I used a simple numerical box model to simulate the δ¹³C excursions of Xiaotan section in a straightforward way. non-steady-state conditions, the time-dependent changing rate of δ^{13} C of marine carbonate is determined by Formula 1. I initiated the forward modeling by giving the uncertain parameters steady-state boundary values (typical Neoproterozoic values). The P4 excursion can be replicated by transiently increasing the amount of organic carbon buried (F_{org}) by 4 fold for a duration of 1 M.yr and keeping for 5 M.yrs and then decreasing back to one tenth of the original F_{org} . These changes in F_{org} could be related to the introduced modern digestion innovations in Phanerozoic time, and the subsequent biological turnover. However, the N1 excursion cannot be replicated by changing F_{org} or M_0 , or both. Instead, it can only be simulated by drastically decreasing δ_w to -13%. Therefore, we must entertain the possibility that there was an isotopically light source of carbon to the surface ocean during the late Neoproterozoic, which could be the release of methane hydrates from an anoxic dissolved organic carbonrich ocean or remineralization of old-time organic matters.

$$\frac{d\delta_0^c}{dt} = \frac{F_w^c(\delta_w^c - \delta_0^c) - F_{org}\Delta_c}{M_0^c}$$
 Formula 1

At the meantime, a backward modeling was tested by starting from the Xiaotan $\delta^{13}C$ profile. Using the best-fitted curve of the isotopic profile and the first-order derivative curve, unrealistic negative F_{org} values was generated, which also implied normal δ_w value could not generate N1.

[1] Li (2013) Prec. Res. 225, 128-147.