INTRODUCTION
With the increased use of dredged materials for building, it has become more important to understand clay mineral behaviour and its impact on sediment strength and stability [1]. Clays, such as montmorillonite (MMT), have been observed to expand in a step-wise fashion when in contact with water in a process called clay swelling [2]. The mechanism underlying such abrupt change of clay thickness and how it affects the stability of sediment are not clear. The aim of this study is to use molecular dynamics to investigate how water adsorption occurs in clay swelling and how clay mineralogy affects this process.

RESULT

• The simulation identifies slow swell from one water layer (1W) to two water layer hydration state (2W) for case Na12 (Fig. 2 (a)), stable 1W state for K12 (Fig. 2 (b)) and a quick swell from 1W to 2W for case Ca6 (Fig. 2 (c)). Step-wise transition is observed for the cases Na12 and Ca6.

• 1W-2W transition is linked to the Na detaching from clay oxygen (Ow) and hydration with water (i.e., bond with Ow), see Fig. 3 (a), (b). As a result, the Ow profile shifts from one peak around Na at 1W state (Fig. 3 (c), (d)) to two peaks around Na at 2W state (Fig. 3 (e)). The relatively lower peaks at higher z position in Fig. 3 (d), (e) are due to the flocculation of the top clay layer.

• Analysis shows a decreasing clay-cation interaction, decreasing hydration capacity and increasing cation migration speed, for Ca, Na and K (Fig. 4). The radial distribution function of cation and Ow supports such descending tendency in hydration capacity.

DISCUSSION & CONCLUSION

• This study reproduced the free swell of MMT layers in clay hydration, in particular, the step-wise 1W-2W transition was captured.
• The mechanism underlying 1W-2W MMT swell is found to be the detachment of cations from the clay surface along with their full hydration.
• The various hydration behavior of Ca, Na- and K-MMT depends on the hydration capacity of the cations as well as the cation migration speed.
• Although the hydration of cation is responsible for the 1W-2W transition, cation provides the dominant attractive force in stabilizing the 1W and 2W hydration states.
• Future work should look into the effect of water chemistry on the swelling behavior of clay, as this can be an important point for the safety use of dredged materials.

REFERENCE