

## **ERICA Modelling workshop**

Wednesday 11<sup>th</sup> July - from 11:00 to Thursday 12<sup>th</sup> July 2018 after lunch, EPFL, Lausanne, Switzerland

Potential participants: Reza Andalibi (PSI), Paul Bowen (EPFL), Dave Faux (Surrey), Sandra Galmarini (Empa), Aslam Kunhi Mohamed (EPFL), Peter McDonald (Surrey), Long Nguyen Tuan (Weimar), Alexandre Ouzia (EPFL), Karen Scrivener (EPFL), Masood Valavi (EPFL), Jigar Parekh (prospective student) and Khalil Ferjaoui (prospective student)

Draft Programme blocks of short presentations focussing on implementation, software, and more followed by discussions

Wednesday 11 <sup>th</sup> July 2018				
	Blocks		Lead	
11:00		Introduction	P. McDonald	
From 11:30	Atomistic level	From atomistic to mesostructures and sorptionthe key questions	P. Bowen	
		The importance of defects, interlayer composition and surfaces at the atomistic level towards understanding gel pore formation	A. Kunhi Mohamed	
		A tool for producing numerical porous microstructures from cylindrical particles	S. Galmarini	
		Discussion		
Lunch				
13:30	Surface and NMR	Linking simulation to NMR	D. Faux	
		Discussion		
Break				
	Meso level	The sheet growth models: current state and technical issues	M. Etzold	
			L. Nguyen Tuan	
		Discussion		
End day 1				
Thursday 12 <sup>th</sup> July 2018				
From 8:30	Kinetics/Microstructure	Modelling the later age hydration kinetics of Alite	A. Ouzia	
		On The Mesoscale Mechanism of Synthetic Calcium-Silicate-Hydrate Precipitation: A Population Balance Modelling Approach	R. Andalibi	



		Discussion		
Break				
	Transport/ LB /		B. Pichler	
		Discussions		
Lunch				
End day 2				