

## **ERICA Modelling workshop**

Wednesday 16<sup>th</sup> January - from 13:45 to Thursday 17<sup>th</sup> January 2019, EPFL, Lausanne, Switzerland Room: Dia004

## Programme

		Wednesday 16 <sup>th</sup> January 2019	
	Blocks		Lead
13:45		Introduction	Fabien /Peter/Paul
14:00		The importance of defects, interlayer composition and surfaces at the atomistic level towards understanding gel pore formation	Aslam Kunhi Mohamed
14:30	- Atomistic level	Zeta potential and distance-dependent diffusivity	Milan Predota
15:15		Sulfate adsorption on cementitious materials	Masood Valavi
15:30		Sulfate adsorption in cementitious materials	Franco Zunino
15:45		Discussion	
16.00 B	reak		,
16:30	Surface and NMR	Linking simulation to NMR – the first MD steps current progress	Dave Faux
17:00	Meso level	Effect of EDL on transport	Ravi Patel
17:30		Chemical activities and potentials across scales	Fabien/Khalil
17:45		Discussion	
End day	18.00		
		Thursday 17 <sup>th</sup> January2018	
8:30		Modelling the later age hydration kinetics of Alite	Alexandre Ouzia
9:00	Kinetics - Microstructure	A Population Balance Modelling Approach to C-S-H precipitation –.the near surface secondary nucleation assumption	Reza Andalibi
9:30		The sheet growth models: current state and future plans	Merlin Etzold
10:00		Discussion	
Break 1	0.30		
11:00		Validation of numerical codes – analytical expressions and experiments – which problems should we solve ?	Peter/Fabien
12:15		Conclusion and plans	Peter/Karen
Lunch 1	2.30		•
End day	2		



## Participant list:

EPFL:

Karen Scrivener, Paul Bowen, Fabien Georget, Masood Valavi, Khalil Ferjaoui, Aslam Kunhi Mohamed, Alexandre Ouzia, Franco Zunino

Surrey:

Peter McDonald, Dave Faux, Arifah Abduris, Miryea Nicole Borg

PSI:

Reza Andalibi, Ravi Patel

TU Wien:

Nabor Segura, Petr Dohnalik

Others:

Merlin Etzold, Milan Predota