Proceedings
PRO 91

CONMOD 2014

Proceedings of the RILEM
International Symposium on Concrete Modelling

Edited by Kefei Li, Peiyu Yan
and Rongwei Yang

RILEM Publications S.A.R.L.

Content

Preface XIX

A. KEYNOTE LECTURES

1. **Microstructural Modelling State of the Art and Perspectives** 3
   Karen L. Scrivener
2. **Quantitative Evaluation Structure of Cement Paste** 4
   Hamlin M. Jennings
3. **Numerical Simulation of Chloride Migration in Concrete Structures under Harsh Environmental Conditions** 5
   Tetsuya Ishida, Yuya Takahashi and Rungrawee Wattanapornprom

B. Hydration & Microstructure

4. **A Combined Kinetic and Thermodynamic Approach for Modelling the Pore Solution of PC-fly Ash Cements** 9
   N. Eroukhmanoff and A. Al-Tabbaa
5. **A Generalized Scale Factor Model for Portland Cement Hydration** 18
   Xueyu Pang
6. **Hydration Kinetics Model of Supersulfated Cement** 27
   Wang Lu, Liu Shuhua, Gao Yuxin and Yu Baoying
7. **Computer Simulation of the Packing of Digitized Reactive Magnesia Particles** 36
   Mingzhi Wang and A. Al-Tabbaa
8. **Simulation of Nano Flow between Calcium Silicate Hydrate Nano Partcles based on Navier-Stokers Equation** 44
   Zhen He, Gengxin Cao and Qiao Zheng
9. **Influence of Microstructural Parameters of Effective Diffusivity of Hydrating Cement Paste** 53
   Neven Ukrainczyk and Eduardus A.B. Koenders
10. **Study on the Effect Particle Size Distribution and Blaine Fineness on the Hydration of Cement** 61
    Shiju Joseph and Shashank Bishnoi

11. Influence of the Particle Size Distribution on Hydration Kinetics: a Mechanistic Analytical Approach **69**

Tulio Honorio, Benoit Bary and Farid Benboudjema

12. Modeling of Hydration of Ultra High Performance Concrete **78**

Xiao-Yong Wang

13. Hydration Simulation of Ternary Blended Cement **87**

Zhijun Tan, Geert De Schutter, Guang Ye, Yun Gao and Lieven Machiels

14. Molecular Dynamics Simulation of Elastic Properties of Tobermorite Family **94**
Shahin Hajilar and Behrouz Shafei

15. A Two-Dimensional Wave Propagation Method for Tortuosity Analysis of Pore Structure **102**

Deqing Xie, Peng Zhao, Lin Yang and Yunsheng Zhang

16. The Influence of Digital Resolution of the Cement Paste Percolation based on CEMHYD3D Model **110**

Cheng Liu and Yunsheng Zhang

17. Numerical Construction of Interfacial Transition Zone around Platonic Particles **118**

Zhigang Zhu and Huisu Chen

C. Shrinkage & Creep

18. Modelling Shrinkage and Thermal Deformations in High Performance of Concrete at Early age **127**

Mateusz Wyrzykowski, Dariusz Gawin and Pietro Lura

19. A Coupled Transport-Reaction Model for Simulating Autogenous Self-healing in Cementitious Materials –Part I: Theory **135**

Haoliang Huang, Guang Ye and Denis Damidot

20. A Coupled Transport-Reaction Model for Simulating Autogenous Self-healing in Cementitious Materials –Part II: Validation **144**

Haoliang Huang, Guang Ye and Denis Damidot

21. Drying and Shrinkage Behaviour of Portland Cement Mortar at Intermediate but Constant Hydration Degree **152**

G. Pham, A. Bauland, A. Delaplace, Q-H. Vu and R. Barbarulo

22. Compressive Strength, Shrinkage and Mass Loss During Simultaneous Hydration and Drying of Concrete: Experimental and Modeling Results **160**

B. Huet, A. Delaplace, G. Pham and R. Barbarulo

23. Early Age Creep and Relaxation Modelling of Concrete under Tension and Compression **168**

B. Delsaute and S. Staquet

24. Homogenization of Solidifying Random Porous Media: Application to Ageing Creep of Cementitious Materials **176**

J. Sanahuja

25. Constitutive Law for the Viscoelastic Behavior of Early Age Concrete in Massive Structures **183**

Wibke Hermerschmidt and Harald Budelmann

26. Drying Shrinkage Effect on Cracking and Structural Strength of Reinforced Concrete Structures **190**

A. Michou, A. Hilaire, C. Desodt, F. Benboudjema, G. Nahas, P.Wyniecki and Y. Berthaud

27. Role of Creep on the Microstructural Damage Induced by Alkali-Silica Reaction **197**

Alain B. Giorla, Cyrille F. Dunant and Karen L. Scrivener

28. Shrinkage Stress Development in Cementitious Materials **204**

Will Hansen, Eduard A.B. Koenders, Zhichao Liu, Bo Meng and Ya Wei

D. Properties

29. Micromechanics of ITZ-Aggregate Interaction in Concrete : Crack Initiation **215**

Markus Königsberger, Bernhard Pichler and Christian Hellmich

30. Numerical Modelling of theWater Isotherms of Cement Paste: Bridging the Gap between the Capillary and C-S-H Gel Pores **222**

M. Zalzale, P.J. McDonald and K.L. Scrivener

31. Nanoindentation Mapping of Mechanical Properties of Cement Paste Blended with Slag **227**

X. Gao and Y. Wei

32. Estimation of Elastic Properties of Cement based Materials at Early Age based on a Combined Numerical and Analytical Multiscale Micromechanics Approach **236**

Tulio Honorio, Benoit Bary and Farid Benboudjema

33. Simulation on Mechanical Behavior of Concrete with Hexagon Recycled Coarse Aggregate in Random Distribution **244**

Xiao Jianzhuang, Lin Zhuangbin, Zhang Kaijian and Sun Chang

34. First-Principles Study of Water Adsorption and Dissociation on β-C_2S (100) Surface **252**

Qianqian Wang, Yanhua Guo, Hegoi Manzano, Iñigo Lopez-Arbeloa, Xiaodong Shen and Feng Li

35. Effect of Microstructural Parameters on Simulation of Mechanical Properties **259**

Shashank Bishnoi, Quang-Huy Do and Karen L. Scrivener

36. Prediction of Water Vapour Sorption Isotherms and Microstructure of Hardened Portland Cement Pastes **265**

James M. de Burgh, Stephen J. Foster and Hamid R. Valipour

37. Simulation of the Development of PH in the Pore Solution of Slag Cement Paste at Early Age **273**

Peng Gao, Guang Ye, Jiangxiong Wei and Qijun Yu

38. Methods for Green Concrete Design **281**

David García, Jorge S. Dolado and José-Tomás San-José

39. Aggregate Shape Effects on the Mechanical Property of Concrete under Tensile Loading: (1) Simulation of One Particle System **290**

Lin Liu, Huisu Chen, Zhigang Zhu and Zhiwei Qian

40. Prediction of Strength of Mortars Containing Fly Ash **297**

Amarpreet Kaur, Shiju Joseph and Shashank Bishnoi

E. Transport

41. 3D Simulation of Cement Paste Aging Due to Reactive Transport **305**

Neven Ukrainczyk and Eduardus A.B. Koenders

42. Inflence of Cracks and Saturation on Mass Transport into Concrete by Mesoscale Computational Method **314**

Wang L.C. and Bao J.W.

43. Capillary Absorption for Cementitious Material considering Water Evaporation and Tortuosity of Capillary Pores **328**

Jinbo Yang, Yue Li, Peng Zhang and Wanguo Dong

44. Modelling of Temperature Impacts on Cement Paste in Clayey Environment Constrained by Field Experiments **335**

Philippines Lalan, Laurent De Windt, Alexandre Dauzères and Valéry Detilleux

45. Modellings of Chloride Ion Transport in Mortars Considering Electrokinetic Behaviors at Pore Walls **343**

Yuya Takahashi , Yogarajah Elakneswaran and Tetsuya Ishida

46. Measuring and Modelling of Water Penetration into Unsaturated Concrete **351**
Peng Zhang, Tiejun Zhao, Jinbo Yang and Congtao Sun

47. Application of a Pore-scale Reactive Transport Model to Study the Influence of Pore Network Characteristics on Calcium Leaching in Cementitious Systems **359**

Ravi A. Patel, Janez Perko, Diederik Jacques, Geert De Schutter, Guang Ye and Klaas Van Breugel

48. Multi-scale Modeling of the Evolution of the Transport Properties of Cement Pastes Subject to Leaching and Carbonation **367**

N. Seigneur, A. Dubus, P.E. Labeau, V. Detilleux, O. Destin and A. Dauzères

49. Micromechanics Modeling the Solute Diffusion in Unsaturated Hardened Cement Paste **374**

Rongwei Yang, Eric Lemarchand, Teddy Fen-Chong and Kefei Li

50. Statistical Study of Existing Chloride Ingress Models in Immersed Concretes **386**

Sylvain Pradelle, Mickaël Thiéry and Véronique Baroghel-Bouny

F. Durability

51. Modeling Kinetics of C-S-H Dissolution during Carbonation of Cement Paste. Beyond the Solid Solution Approach **401**

Patrick Dangla, Antoine Morandeau and Mickael Thiéry

52. Accelerated Carbonation Modelling of Fly Ash Blended Cement Paste **408**

A. Morandeau, M. Thiéry, P. Dangla and C.E. White

53. Modeling Sulfate Attack in Concrete using Mixture Theory **417**

Chethan Gouder and U. Saravanan

54. Modelling of H2S Attack of Concrete in Sewer Pipes **425**

Haifeng Yuan, Patrick Dangla, Huisu Chen, Patrice Chatellier and Thierry Chaussadent

55. Multiscale Modeling of Alkali Silica Reaction Degradation of Concrete **432**

Gianluca Cusatis, Mohammed Alnaggar and Roozbeh Rezakhani

56. Predicting Depth of Carbonation of Concrete - a Performance-based Approach **440**

Rakesh Gopinath, Mark Alexander and Hans Beushausen

57. Research of the Failure Process of Concrete under the Effect of Freezing-Cycle by Thawing Using X-Ray Industrial CT Technique **448**

J. Yuan, Y. Liu, B.K. Zhang and H.X. Li

58. Thermo-Hydro-Ionic Transport through an Immerged Tube Tunnel for a Service Life of 120 years **453**

Xiaoyun Pang, Kefei Li and Patrick Dangla

59. A New Model for the Calculation of Structures Affected by DEF Application to a Viaduct Case **461**

O. Omikrine-Metalssi, B. Kchakech, S. Lavaud, B. Godart and F. Beauvallet

60. Corrosion-Induced Bond Deterioration in Reinforced Concrete Structures **471**

Shangtong Yang and Chun-Qing Li

61. Mesoscale Simulation of Damage for Mortar and Concrete during Freeze-Thaw cycles **479**

Fuyuan Gong, Yi Wang, Tamon Ueda and Dawei Zhang

62. Concrete Sorptivity as a Performance-based Criterion for Salt Frost Scaling Resistance **487**

Zhichao Liu, Will Hansen and Ya Wei

63. MC Simulation of Reliability Sensitivity Analysis for Marine Concrete Structures Based on FVM **497**

Xingang Zhou, Erju Li and Kefei Li

64. Mechanical Modeling of Chemo-Mechanical Coupling Behavior of Leached Concrete **505**

Bei Huang, Chunxiang Qian and Shao Jianfu

METHODS FOR GREEN CONCRETE DESIGN

David García (1), Jorge S. Dolado (1) and José-Tomás San-José (2)

(1) TECNALIA Research & Innovation, Spain

(2) University of the Basque Country. Engineering Materials Dep., Spain

Abstract

Concrete is the most widely used construction material in the world and causes a substantial environmental impact, mainly during cement manufacture. Portland cement contributes greenhouse gases both directly through the production of carbon dioxide when calcium carbonate is thermally decomposed, producing lime and carbon dioxide, and also through the use of energy, particularly from the combustion of fossil fuels. The use of superplasticizers and blended cements as well as optimization of particle-size distribution and reduction in water content allows a significant reduction in Portland cement clinker in the concrete.

As the demand for eco-friendly construction spreads over developed countries, it is necessary to increase and quantify the contribution of concrete to the environmental sustainability.

Accordingly, several methods for environmental sustainable assessment are presented and discussed in this paper. A lack of consensus about the most adequate impact criteria to be considered is observed. Simplified indexes combined with public life-cycle inventories require a minimum effort and can be useful as a first evaluation of concrete formulations or OCP replacement by supplementary cementitious materials. However accurate comparisons and new low-energy embodied cements evaluations can only be performed through a detailed review of all the materials and processes involved in the life cycle of the concrete.

1. INTRODUCTION

About 25 billion tons of concrete are produced each year in the world, making concrete the most widely used construction material [1]. Concrete demand and production is expected to increase 2.5 times between 2005 and 2050 [2]. The largest share of this growth will take place in China, India and other developing countries on the Asian continent [3]. Concrete causes a substantial environmental impact, mainly during cement manufacture, because of such huge quantities [4].

Concrete is manufactured from hydraulic cement, aggregates and water. It usually contains a small amount of some chemical admixture and it often contains a mineral admixture replacing some part of the cement. Most of these constituents are themselves manufactured products, byproducts or materials extracted by mining. In order to assess the

The definition of a performance indicator (e.g. compressive strength) allows comparing the efficiency of concretes with different performances which in turn collaborates in the search for an optimum mix design.

Simplified indexes as cement or binder intensity combined with updated life-cycle inventories require a minimum effort and can be useful as a first evaluation of concrete formulations or OCP replacement by supplementary cementitious materials. Nevertheless accurate comparisons and new low-energy embodied cements evaluations can only be performed through a detailed review of all the materials and processes involved in the life cycle of the concrete.

ACKNOWLEDGEMENTS

This research work is possible thanks to financing support of Green Concrete Research group (TECNALIA) and the Basque Regional Government research group IT781-13.

REFERENCES

[1] T. Proske, S. Hainer, M. Rezvani, C.A. Graubner. Eco-friendly concretes with reduced water and cement contents — Mix design principles and laboratory tests. *Cement and Concrete Research* 51 (2013) 38–46

[2] Müller N, Harnisch J. A blueprint for a climate friendly cement industry. Gland: *WWF Lafarge conservation partnership*; 2008. p. 94 (WWF – Lafarge conservation partnership report).

[3] The cement sustainability initiative (CSI). The cement sustainability initiative; 2007. p. 8 (*CSI report*). http://www.wbcsdcement.org

[4] J.M. Crow. The concrete conundrum. *Chemistry World*. March 2008 62-66

[5] Lasserre P. The global cement industry, global strategic management mini cases series. *Globalisation Cement Industry* 2007.

[6] Brundtland Commission (1987). Report of the World Commission on Environment and Development. *United Nations*.

[7] Scerri, Andy; James, Paul (2010). "Accounting for sustainability: Combining qualitative and quantitative research in developing 'indicators' of sustainability". *International Journal of Social Research Methodology* 13 (1): 41–53. doi:10.1080/13645570902864145.

[8] San-Jose Lombera JT, Garrucho I, Losada R, Cuadrado J. A proposal for environmental indicators towards industrial building sustainable assessment. *International Journal of Sustainable Development and World Ecology* 2007;14(2):160-173.

[9] United Nations Environment Programme. 2013 Annual Report. ISBN: 978-92-807-3380-8

[10] Goñi S. et al.; Quantitative study of hydration of C_3S and C_2S by thermal analysis: Evolution and composition of C-S-H gels formed. *Journal of Thermal Analysis and Calorimetry* 102 (3): 965-973

[11] Hernández M. S. et al. Synergy of T1-C 3S and β-C_2S Hydration Reactions. *Journal of the American Ceramic Society* 94 (4) : 1265-1271

[12] Goñi S. et al. 2011; Textural and mechanical characterization of C-S-H gels from hydration of synthetic T1-C 3S, β-C 2S and their blends. *Materiales de Construccion* 61 (302): 169-183

[13] J. S. Dolado. Computationally driven design of cement-based materials. Nanotechnology and Sustainability in Construction. *Proceedings of the FraMCoS-8/30GEF Workshop*, Coordinated by S. P. Shah ; S. P. Shah, G. Ruiz, R. C. Yu, X.X. Zhua & C. Andrade (Eds).

[14] Palomo A, Grutzeck MW, Blanco MT. (1999). Alkali-activated fly ashes - A cement for the future. *Cement & Concrete Research* 29(8), 1323-1329. http://dx.doi.org/10.1016/S0008-8846(98)00243-9