

**PREDICTION OF TEMPERATURE RISE IN CONCRETE
DUE TO HEAT OF HYDRATION OF CEMENT**

Anura I.G.K. Mataraarachchi

(09/8103)

Degree of Master of Philosophy

Department of Civil Engineering

University of Moratuwa

Sri Lanka

March 2016

**PREDICTION OF TEMPERATURE RISE IN CONCRETE
DUE TO HEAT OF HYDRATION OF CEMENT**

Anura I.G.K. Mataraarachchi

(09/8103)

Thesis submitted in fulfillment of the requirements for the degree Master of
Philosophy in Civil Engineering

Department of Civil Engineering

University of Moratuwa

Sri Lanka

March 2016

Declaration

I declare that this is my own work and this thesis does not incorporate without acknowledgement any material previously submitted for a Degree or Diploma in any other University or institute of higher learning and to the best of my knowledge and belief it does not contain any material previously published or written by another person except where the acknowledgement is made in the text.

Also, I hereby grant to University of Moratuwa the non-exclusive right to reproduce and distribute my thesis, in whole or in part in print, electronic or other medium. I retain the right to use this content in whole or part in future works (such as articles or books).

Signature

Date

The above candidate has carried out research for the MPhil thesis under our supervision.

Name of the supervisor

Signature of the supervisor

Date

Name of the co supervisor

Signature of the co supervisor

Date

Abstract

Temperature rise due to heat of hydration in concrete depends on many factors such as geometry of the concrete element, chemical, physical and thermal properties of concrete materials, mix proportion, initial temperature during concrete batching, and thermal boundary conditions during concrete hardening etc. The multicomponent cement hydration model developed by Maekawa et al., predicts the heat generation due to cement hydration based on cement contents, water contents, reference heat generation rate of main mineral components in cement, i.e. alite (C_3S), belite (C_2S), aluminate (C_3A), ferrite (C_4AF), and gypsum (CS_2H), mineral of cement, fineness of cement, thermal activity and interdependences of mineral components, and effects of consumption of free water during the hydration process etc. This cement hydration model was incorporated in the transient heat conduction analysis. The transient heat conduction analysis was carried out with ANSYS, finite element analysis software using Advance Parametric Design Language (APDL) computer programming to predict the temperature rise due to heat of hydration of cement in concrete element for a given thermal boundary conditions.

Since the heat of hydration of cement is highly temperature dependent, variation of thermal properties of concrete at early ages is essential to predict the temperature response due to heat of hydration of cement in concrete. Experimental investigations were carried out to develop a model to estimate the variation of thermal conductivity of concrete from fresh to hardened state. The specific heat capacity of concrete (c) was estimated based on the specific heat capacities of cement powder and hydration products using Dulong – Petit Rule (DPR), Neumann – Kopp Rule (NKR), and mixing theory. Thermal conductivity of concrete (λ) was determined by fitting temperature rise curve at center of cube with temperature rise curve predicted by transient heat conduction analysis. Estimated specific heat capacity of concrete was applied in

transient heat conduction analysis program, to predict temperature rise curve from 1hrs to 1day for several mix proportions.

A mathematical model was developed to predict the variation of thermal conductivity based on experimentally investigated thermal conductivity data, mix proportions, thermal conductivity of concrete material found in literature, cement and water contents, formation, shapes, and saturation of gel and capillary pores of cement paste, degrees of hydration, surface saturation of aggregates by applying into general and effective medium theories used in estimation of effective thermal conductivity of a multicomponent material. The developed model was calibrated and verified with experimental data of concrete cube samples for several mix proportions. A computer program was developed using APDL coding of ANSYS software to predict the thermal properties of concrete once mix proportion, chemical, physical and thermal properties of concrete materials are known. This model was coupled with the multicomponent heat of hydration model to improve the program's ability to predict temperature rise with effects of variation of thermal properties with degree of hydration of cement.

The developed multicomponent heat of hydration model was calibrated and verified with temperature rise data obtained from several field tests which were carried out in several construction projects in Sri Lanka. Measured and predicted temperature response are in good agreement, and therefore the proposed model can be used to predict temperature rise when chemical composition, mix proportions, and thermal boundary conditions are known.

Furthermore, the developed hydration model was used to obtain appropriate values for T_1 (i.e. temperature drop between hydration peak and ambient temperature under local conditions which are required in design of water retaining structures).

Keywords: heat of hydration, thermal conductivity, specific heat capacity, early age concrete, transient heat conduction analysis.

This thesis is dedicated

To my Parents, Loving Wife and Son

Without whom none of my success would be possible

Acknowledgement

First, I would like to thank my main supervisor, Prof. S.M.A. Nanayakkara, and co-supervisor, Prof. Shingo Asamoto, who have guided me these last six years. I sincerely appreciate their continuous support, generosity and advice in both academic and personal way throughout my MPhil study. Under their guidance, I successfully overcame many difficulties and learned a lot. This achievement in my life would not have been possible without their guidance, support and encouragement.

Also, I would like to thank the faculty of engineering specifically those in the Department of Civil Engineering who have contributed to my education or aided me in my research. I am especially grateful to Dr. Mrs. Premini Hettiarachchi for the initial encouragement to start this research degree, once I successfully completed my post graduate diploma in Structural Engineering Designs.

I greatly appreciate for the assistance that I received from the staff of the Materials Testing Laboratory. Without their support and technical knowledge, I would not able to complete experimental investigation works of my research.

Specially, I greatly acknowledge HOLCIM Lanka about their financial assistance to carry out experimental investigations to initial verifications, and calibrations of the research outcomes.

Last, but certainly not least, I would like to thank my family for the love and support they showed me along this journey. This includes my father, mother, and wife, who pushed me the most and always encouraged me to work harder when it got tough. I do not consider this achievement to be my sole accomplishment but instead one that I share with them.

Table of Content

Declaration.....	ii
Abstract.....	iii
Dedication.....	vi
Acknowledgement.....	vii
Table of Content.....	viii
List of Figures.....	xii
List of Tables.....	xvi
List of Symbols.....	xviii
1 Introduction.....	1
1.1 Background.....	1
1.2 Objectives.....	3
1.3 Outline of Thesis.....	4
2 Literature Review.....	7
2.1 Introduction.....	7
2.2 Ordinary Portland Cement.....	7
2.3 History of Studies on Heat Generation Associated with Cement Hydration	
12	
2.4 Thermal Cracking.....	15
2.5 Microstructure of Concrete.....	15
2.6 Cement Hydration.....	18
2.7 Parameters Influence the Cement Hydration.....	22
2.8 Modelling of Heat of Hydration of cement.....	27
2.9 Thermal Properties of Concrete.....	29
3 Methodology.....	33
3.1 Introduction.....	33

3.2	Transient Heat Conduction Analysis	34
3.3	Modelling of Heat of Hydration of Cement.....	41
3.4	Modeling of Specific Heat Capacity of Concrete	51
3.5	Modeling of Thermal Conductivity of Concrete	56
3.6	Modeling Initial and Thermal Boundary Conditions.....	63
4	Experimental Investigations.....	72
4.1	Introduction.....	72
4.2	Objective	72
4.3	Experimental Program	73
4.4	Ordinary Portland cement Types	74
4.5	Fine and Coarse Aggregates	76
4.6	Physical and Thermal Properties of Material, and Thermal Boundary Parameters.....	76
5	Experimental Investigation of Thermal Properties of Concrete.....	79
5.1	Introduction.....	79
5.2	Sensitivity Analysis	79
5.3	Experimental Setup.....	81
5.4	Heat Conduction Analysis to Estimate Thermal Conductivity of Concrete.....	84
5.5	Experimental Plan.....	85
5.6	Specific Heat Capacity of Concrete.....	86
5.7	Thermal Conductivity of Concrete	86
5.8	Summary	88

6	Experimental Investigation of Temperature Rise in Concrete due to Heat of Hydration of Cement	90
6.1	Introduction.....	90
6.2	Experimental Setup.....	90
6.3	Experimental Plan.....	93
6.4	Experimental Results	94
6.5	Summary	97
7	Calibration and Verification of Simulation Program	98
7.1	Introduction.....	98
7.2	Thermal Conductivity Model.....	98
7.3	Thermal Analysis by FEM.....	105
7.4	Initial Calibration with Experimental Data from Test Block BLK 01	106
7.5	Initial Verification with Experimental Data from Test Block BLK 02	109
7.6	Further Verification with Temperature Rise Data from Previous Field Investigation.....	112
8	Applications of Developed Model	118
8.1	Effects of Variation of Mineral Composition	118
8.2	Recommendations for T_1	120
9	Discussion & Conclusions	124
10	Recommendations	126
	References	127
	APPENDIX A : APDL Codes of Geometric Model	xx
	APPENDIX B : APDL Codes of Parameter Inputs	xxviii
	APPENDIX C : APDL Codes of Heat Conduction Analysis Program.....	xxxv
	APPENDIX D : APDL Codes of Subroutine to Estimate Heat of Hydration.....	xlvi
	APPENDIX E : APDL Codes of Subroutine to Set Specific Heat Capacity of Concrete.....	xcvii

APPENDIX F : APDL Codes of Subroutine to Set Thermal Conductivity of Concrete.....	xcviii
APPENDIX G : APDL Codes of Subroutine to Set Ambient Temperature	cii
APPENDIX H : APDL Codes of Program to Investigate Thermal Conductivity of Concrete.....	ciii
APPENDIX I : Outputs of Thermal Conductivity Model	cvi

List of Figures

Figure 2-1: Microstructure of different clinker polymorphs	8
Figure 2-2: Component of concrete.....	16
Figure 2-3: General stages of exothermic hydration process in OPC	18
Figure 2-4: Chemical reactions during initial stage of cement hydration [53].....	19
Figure 2-5: C ₃ A Grain after 10min Hydration with the Presence of Calcium Sulfate	20
Figure 2-6: Increasing the permeability of semi stable CSH, and ettringite layer at termination of dormant period [53]	21
Figure 2-7: SEM Photograph of C-S-H.....	21
Figure 2-8: Chemical reaction process during acceleration and deceleration periods of cement hydration process	22
Figure 2-9: Adiabatic Temperature Rise in Mass Concrete for Different Cement Types	23
Figure 2-10: Variation of Instant Heat of Hydration Rate against Sulfate Content ..	24
Figure 2-11: Rate of heat generation as affected by Wagner fineness of cement (ASTM C 115) for cement paste cured at 75 °F (23.8 °C).....	25
Figure 2-12: Effects w/c ration on Heat of Hydration Rate in cement.....	26
Figure 2-13: Effects of Curing Temperature on cement Hydration [63].....	27
Figure 3-1: Flow Chart for Heat Conduction Analysis	36
Figure 3-2: Reference heat generation curves for formation of hydrates and mono-sulfate at reference temperature, T ₀ = 293 K.....	43
Figure 3-3: Reference heat generation rate curves for formation of ettringite at reference temperature, T ₀ = 293 K	43
Figure 3-4: Reference heat generation rate curves for Slag & Fly ash reaction at reference temperature, T ₀ = 293 K	44
Figure 3-5: Thermal activity on reaction of cement minerals	45
Figure 3-6: Flow Chart to Estimate Heat Generation Rate due to Cement Hydration	50
Figure 3-7: Flow Chart to Estimate Specific Heat Capacity of Concrete	56
Figure 3-8: Flow Chart to Estimate Effective Thermal Conductivity of Concrete ...	62

Figure 3-9: Angle used to calculate solar incidence angle on concrete surface	68
Figure 3-10: Flow Chart to Estimate Thermal Boundary Conditions	71
Figure 5-1: Sensitivity of Temperature Response to Specific Heat Capacity of Concrete.....	81
Figure 5-2: Experimental setup to measure internal temperature rise of specimens using a hot water bath.....	82
Figure 5-3: Specimens are inside Hot Water Bath	82
Figure 5-4: Specimen geometry, dimensions, and boundary conditions.....	83
Figure 5-5: Concrete Specimens Out Side the Hot Water Bath	83
Figure 5-6: Data Logger	84
Figure 5-7: Fitted temperature response curves with relevant experimental data of M-3 specimen 1 & 2	87
Figure 5-8: Variation of Thermal Conductivity of Concrete Mixes.....	88
Figure 6-1: Experimental Setup to Measure Temperature Rise Due to Heat of Hydration of Cement	91
Figure 6-2: Geometry and Locations of Thermocouples for Concrete Test Block BLK 01	91
Figure 6-3: Geometry and Locations of Thermocouples for Concrete Test Block BLK 02	92
Figure 6-4: Temperature Rise and Ambient Temperature Variation with Time - Test Block BLK 01.....	95
Figure 6-5: Temperature Rise and Ambient Temperature Variation with Time - Test Block BLK 02.....	96
Figure 7-1: Variation of Fractional Volumes of each components in Cement Paste for mix M-2 during initial stages.....	99
Figure 7-2: Variation of Degrees of Hydration [DoH] for mix M-2 during initial stages	101
Figure 7-3: Variation of shape factor for solid and gas phases in cement paste [$d_{s\&g}$] for mix M-2 during initial stages.....	101
Figure 7-4: Variation of thermal conductivity of water and vaporized air in pores of cement paste of mix M-2 during initial stages	102
Figure 7-5: Variation of Thermal Conductivity of Cement Paste, Mortar, and Concrete for mix M-2.....	104

Figure 7-6: Experimentally Investigated and Predicted Variation of Thermal Conductivity of Concrete Mixes M-1, M-2, and M-3	105
Figure 7-7: Variation of Thermal Conductivity of Concrete Mix M-4 Predicted by Thermal Conductivity Model	106
Figure 7-8: Plan View - Geometric Orientation of Test Block BLK 01	107
Figure 7-9: Picture from Thermal Analysis of BLK 1 using ANSYS	108
Figure 7-10: Temperature Rise and Ambient Temperature Variation Predicted and Measured from Test Block BLK 01	109
Figure 7-11: Variation of Thermal Conductivity of Concrete Mix M-5 Predicted by Thermal Conductivity Model	110
Figure 7-12: Plan View - Geometric Orientation of Test Block BLK 02	111
Figure 7-13: Picture from Thermal Analysis of BLK 2 using ANSYS	111
Figure 7-14: Temperature Rise and Ambient Temperature Variation Predicted and Measured from Test Block BLK 02	112
Figure 7-15: Temperature Rise and Ambient Temperature Variation Predicted and Measured from 300mm Thick Wall in Project 1.....	115
Figure 7-16: Temperature Rise and Ambient Temperature Variation Predicted and Measured from 500mm Thick Wall in Project 2.....	116
Figure 7-17: Temperature Rise and Ambient Temperature Variation Predicted and Measured from 750mm Thick Wall in Project 3.....	116
Figure 8-1: Predicted Adiabatic Temperature Rise for OPC Products Available in Local Market.....	119
Figure I-1: Variation of Fractional Volumes of each components in Cement Paste for mix M-1 during initial stages	cvi
Figure I-2: Variation of Fractional Volumes of each components in Cement Paste for mix M-3 during initial stages	cvi
Figure I-3: Variation of Degrees of Hydration [DoH] for mix M-1 during initial stages	cvii
Figure I-4: Variation of Degrees of Hydration [DoH] for mix M-3 during initial stages	cvii
Figure I-5: Variation of shape factor for solid and gas phases in cement paste [$d_{s\&g}$] for mix M-1 during initial stages.....	cviii

Figure I-6: Variation of shape factor for solid and gas phases in cement paste [$d_{s\&g}$] for mix M-3 during initial stages	cvi
Figure I-7: Variation of thermal conductivity of water and vaporized air in pores of cement paste of mix M-1 during initial stages	cix
Figure I-8: Variation of thermal conductivity of water and vaporized air in pores of cement paste of mix M-3 during initial stages	cix
Figure I-9: Variation of Thermal Conductivity of Cement Paste, Mortar, and Concrete for mix M-1	cx
Figure I-10: Variation of Thermal Conductivity of Cement Paste, Mortar, and Concrete for mix M-3	cx

List of Tables

Table 2-1: Oxides in Ordinary Portland cement.....	9
Table 2-2: Bouge Equations to Convert Oxide Composition into Mineral Composition in OPC.....	10
Table 2-3: ASTM C150 Standard Requirements for OPC and Blended Cements....	11
Table 2-4: EN197-1 and BS8500 Standards for OPC & Blended Cements.....	12
Table 3-1: User defined system of units uses in thermal analysis.....	35
Table 3-2: List of arrays used to store and retrieve data during thermal analysis.....	37
Table 3-3: Physical and thermal properties of material uses in thermal analysis	39
Table 3-4: Atomic Heat for Solid Elemental Substances	52
Table 3-5: Specific Heat Capacities of Cement Mineral Components.....	53
Table 3-6: Specific Heat Capacities of Cement Hydration Products	54
Table 3-7: Heat flow constant, C for different surface orientations.....	67
Table 3-8: Equation of time based on Julian day of the year	70
Table 4-1: Chemical Compositions of Cement Types.....	74
Table 4-2: Weight Percentage of Mineral Components of OPC.....	75
Table 4-3: Physical Properties of OPC Cement Types	76
Table 4-4: Physical and Thermal Properties of Concrete, Formwork, and Insulations Material.....	77
Table 4-5: Emissivity, and Absorptivity, for Material used in Heat Conduction Analysis	78
Table 4-6: Coefficient of Thermal Convection for Material Surfaces	78
Table 5-1: Selected Specific Heat Capacity of Concrete assuming Thermal Conductivity as a Constant.....	80
Table 5-2: Concrete Mix Proportions.....	85
Table 5-3: Estimated Specific Heat capacity of Concrete for three Concrete Mixes	86
Table 6-1: Concrete Mix Proportions.....	93
Table 6-2: Maximum Temperature at Center & Insulated Faces, and Time of Concreting - Test Block BLK 01	96

Table 6-3: Maximum Temperature at Center & Faces, and Time of Concreting - Test Block BLK 02.....	97
Table 7-1: Phases and Shapes of Components in Cement Paste	100
Table 7-2: Details of Field Test.....	113
Table 7-3: Concrete Mix Proportions used in Field Test	114
Table 7-4: Thermal and Physical Properties Predicted by the model for Concrete Mixes used in Field Test.....	114
Table 7-5: Summary of Measured and Predicted Maximum Temperatures and Time to Reach the Maximum Temperature for each Field Test.....	117
Table 8-1: Chemical Composition of OPC Available in Local Market	118
Table 8-2: Mineral Composition, Powder Fineness, and Equivalent ASTM and European Cement Types of OPC Available in Local Market Products	119
Table 8-3: T ₁ Values for Different Wall Thickness and Formwork Materials.....	122

List of Symbols

Latin Symbols

OPC	Ordinary Portland Cement
APDL	Advance Parametric Design Language
THW	Transient Hot Wire
TLS	Transient Line Source
THS	Transient Hot Strip
TPS	Transient Plane Source
C	Carbon
Mg	Magnesium
Al	Aluminum
Fe	Ferrous
Si	Silicon
Ca	Calcium
C ₃ S	3CaO.SiO ₂ - Alite
C ₂ S	2CaO.SiO ₂ - Belite
C ₃ A	3CaO.Al ₂ O ₃ - Aluminate
C ₄ AF	4CaO.Al ₂ O ₃ .Fe ₂ O ₃ - Ferrite
CSH	Calcium Silicate Hydrates
CS ₂ H	Gypsum
AEt & FEt	Ettringite
CH	Calcium Hydroxide
LH	Low Heat
SR	Sulfate Resistant
DPR	Dulong-Petit Rule
NKR	Neumann - Kopp Rule
HS	Hashin-Strikman Bound Theorem
MM	Maxwell Model
MEL	Maxwell – Eucken Limits
EMT	Effective Medium Theory
DoH	Degrees of Hydration
T ₀	Temperature at 0 K
T ₁₀₀	Temperature at 100 K
Q _R	Volumetric Heat Generation Rate
K	Thermal Conductivity
K ₀	Thermal Conductivity of Concrete at 0 K
K ₁₀₀	Thermal Conductivity of Concrete at 100 K
M	Fractional Mass
X	Molar Fraction

P	Pressure
V	Volume
W	Weight
A	Area
Q	Heat Flow
T_s	Surface Temperature
T_a	Ambient Temperature
NLS	Number of Time Intervals
H_c	Specific Heat Generation Rate for Cement Powder
p	Fractional Mass of Cement Minerals
Q_i	Accumulated Heat
R	Gas Constant
E/R	Thermal Activity
T	Temperature
s_i	Fineness of Cement Powder
S_i	Blaine Value of Cement Minerals
S_{io}	Reference Blaine Value of Cement Minerals
WC	Unite Weight of Cement
P3A	Weight Percentage of Aluminate
P3S	Weight Percentage of Alite
P4AF	Weight Percentage of Ferrite
P2S	Weight Percentage of Belite
PPCS2H	Weight Percentage of Gypsum
PPC	Weight Percentage of OPC
BLN	Blaine Value of OPC
PSG	Weight Percentage of Slab
BLNSG	Blaine Value of Slag
SGCS2H	Weight Percentage of Sulfate in Slag
PFA	Weight Percentage of Fly Ash
BLNFA	Blaine Value of Fly Ash
FACS2H	Weight Percentage of Sulfate in Fly Ash
PLS	Weight Percentage of Superplasticizer
BLNLS	Blaine Value of Superplasticizer
WP	Water to Powder Ratio
QSP	Constant for the Effects of Superplasticizer Dosage
QSPAD	Constant for the Effects of Superplasticizer Dosage
CHARSP	Constant for the Effects of Superplasticizer Dosage
QSGMX	Final Accumulated Heat Generated by Slag
RSGW1	Weight Percentage of Consumed Water of by Slab
RSGCA	Weight Percentage of Consumed Calcium

QFAMX	Hydroxide when reacts with Slag
RFAW1	Final Accumulated Heat Generated by Fly Ash
RFACA	Weight Percentage of Consumed Water by Fly Ash
	Weight Percentage of Consumed Calcium
	Hydroxide when reacts with Fly Ash
RH3AMN	Factor for Mono-sulfate Conversion
w	Velocity of Wind
h	Convection Coefficient
E_N	Solar Radiation on Horizontal Surface
E_V	Solar Radiation on Vertical Surface
L_a	Latitude
L_o	Longitude
LST	Local Standard Time
LSM	Local Standard Time Meridian
q	Heat Flux
T_{dp}	Dew Point

Greek Symbols

c	Specific Heat Capacity of Concrete
ρ	Density of Concrete
γ	Retarding effects of fly ash and admixture
β	Free water content
μ	Effects of weight percentage of clinker minerals
λ	Effects of calcium hydroxide production on reaction
of fly and slag	
\emptyset	Porosity
δ	Solar Declination Angle
σ	Stefan – Boltzmann Constant
ϵ	Emissivity
α	Thermal Diffusivity

Subscript

i, j, k	Counters
t	Time
x, y, z	Directions