MULTISCALE MICROMECHANICAL MODELLING OF THE INFLUENCE OF INTERFACIAL TRANSITION ZONE ON THE MECHANICAL AND TRANSPORT PROPERTIES OF CEMENTITIOUS MATERIALS

MEENAKSHI SHARMA

DEPARTMENT OF CIVIL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY DELHI
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by

Meenakshi Sharma
DEPARTMENT OF CIVIL ENGINEERING

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CERTIFICATE

This is to certify that the thesis entitled “MULTISCALE MICROMECHANICAL MODELLING OF THE INFLUENCE OF INTERFACIAL TRANSITION ZONE ON THE MECHANICAL AND TRANSPORT PROPERTIES OF CEMENTITIOUS MATERIALS”, being submitted by Ms. Meenakshi Sharma, to the Indian Institute of Technology Delhi, for the award of the degree of ‘Doctor of Philosophy’ in Department of Civil Engineering is a record of the bonafide research work carried out by her under our supervision and guidance. She has fulfilled the requirements for submission of this thesis, which to the best of our knowledge has reached the requisite standard.

The material contained in the thesis has not been submitted in part or full to any other University or Institute for the award of any other degree or diploma.

(Prof. Shashank Bishnoi)
Associate Professor
Department of Civil Engineering
Indian Institute of Technology Delhi

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ABSTRACT

The interfacial transition zone (ITZ) between cement paste and aggregate is a weak and porous interface in concrete whose influence on the properties of concrete has been a subject of debate. It was long accepted as the weakest link in concrete, however doubts have also shown on this conventionally accepted concept. In addition to the ITZ, different heterogeneities present at different scales of concrete influence its behaviour at the structural scale. A shift from utilization of natural materials to waste materials such as supplementary cementitious materials, construction and demolition waste, etc. leads to an increase in these heterogeneities. A better understanding of the influence of various heterogeneities on the properties of concrete is crucial for its optimum design.

The objective of this study was to investigate the influence of these heterogeneities on the overall behaviour of concrete. A combination of experimental and analytical modelling studies was carried out to better understand the behaviour of aggregates, interfacial transition zone and fly ash on the properties of concrete. Ultrasonic pulse velocity test and sorptivity test were performed to measure the elastic and transport properties. A new multiscale continuum micromechanics-based approach was developed to model the mechanical and transport properties of concrete incorporating the microstructure of interfacial transition zone. The multiscale nature was incorporated in the approach from the scale of C-S-H gel to the scale of concrete. The microstructure of ITZ around aggregates was simulated using µic, a cement microstructural hydration model. The gradients in the microstructure of ITZ were addressed by homogenizing it in thin layers starting from the surface of aggregate to the bulk cement paste.

The experimental studies demonstrated that the influence of ITZ on elastic modulus, compressive strength and transport properties is complex and that modelling is necessary to distinguish the influence of ITZ from other effects. The experimental study also indicated that the increased presence of fly ash particles in the ITZ leads to an improvement in the mechanical properties of mortars compared to pastes. It was observed that the microstructure of ITZ could be simulated around large particles in a computational volume using the cement hydration model. The modelling studies showed that the large gradients within the microstructure of ITZ is the controlling factor for the compressive strength of concrete. Its influence on the transport properties was found to be higher compared to the influence on elastic properties. The modelling study also demonstrated that why the experimental studies usually conducted to understand the influence of ITZ does not capture the influence of ITZ on the overall behaviour of concrete. The modelling results provide insights into the influence of fly ash on the development of compressive strength. It was seen that pozzolanic reaction of fly ashes leads to an increase in the C-S-H content in the C-S-H foam, especially in the ITZ, allowing the mortars to gain strengths similar to those without fly ash, despite having a higher total porosity. It was also observed that the changes in the composition of C-S-H, usually observed experimentally, may influence the phase assemblage but its influence on the elastic properties of mortars is little.

सार

सीमेंट पेस्ट और गिट्टी के बीच सीमा परिवर्तन क्षेत्र (आई.टी.जेड.) कंक्रीट का एक कमजोर अंश है जिसका कंक्रीट के गुणों पर प्रभाव बहस का विषय रहा है। यह लंबे समय से कंक्रीट में सबसे कमजोर कड़ी के रूप में स्वीकार किया गया था, हालांकि इस पारंपरिक रूप से स्वीकृत अवधारणा पर संदेह भी दिखाया गया है। आई.टी.जेड. के अलावा, कंक्रीट के विभिन्न स्तर पर मौजूद विभिन्न विषमताएँ इसके व्यवहार को प्रभावित करती हैं। प्राकृतिक सामग्री के स्थान पर अन्य अपशिष्ट पदार्थ, जैसे कि पूरक सिमेंट सामग्री, निर्माण विध्वंस सामग्री, अत्यादि के उपयोग के कारणवश कंक्रीट की विषमताओं में वृद्धि होती है। कंक्रीट के गुणों पर विभिन्न विषमताओं के प्रभाव का बेहतर ज्ञान इसके इष्टतम रचना के लिए महत्वपूर्ण है।

इस अध्ययन का उद्देश्य कंक्रीट के समग्र व्यवहार पर इन विषमताओं के प्रभाव की जांच करना था। कंक्रीट के गुणों पर समुच्चय, आई.टी.जेड. और फ्लाई ऐश के व्यवहार को बेहतर ढंग से समझने के लिए प्रयोगात्मक और विश्लेषणात्मक मॉडलिंग अध्ययनों का एक संयोजन किया गया था। लचीलेपन और परिवहन गुणों को मापने के लिए अल्ट्रासोनिक पल्स वेलोसिटी टेस्ट और सॉरप्टिविटी टेस्ट किया गया। आई.टी.जेड. के सूक्ष्म संरचना को शामिल करते हुए कंक्रीट के लचीलेपन और परिवहन गुणों को मॉडल करने के लिए एक नया बहुमपिया कंटिनयुआम सूक्ष्म-यांत्रिकी -आधारित दृष्टिकोण विकसित किया गया था। बहुमपिया प्रकृति को सी-एस-एच जैल के पैमाने से कंक्रीट के पैमाने तक के दृष्टिकोण में शामिल किया गया था। गिट्टियों के आसपास आई.टी.जेड. के सूक्ष्म संरचना को माइक, जो कि एक सीमेंट सूक्ष्म संरचना जल योजन मॉडल है, का उपयोग करके अनुकरण किया गया था। आई.टी.जेड. की सूक्ष्म संरचना में विषमताओं को गिट्टियों की सतह से लेकर मध्यम सीमेंट पेस्ट तक पतली परतों में समरूप बनाकर संबोधित किया गया था।

प्रायोगिक अध्ययनों से पता चला है कि लचीलेपन, मज़बूती और प्रसरणीयता पर आई.टी.जेड. का प्रभाव जटिल है और आई.टी.जेड. के प्रभाव को अन्य प्रभावों से अलग करने के लिए मॉडलिंग आवश्यक है। प्रायोगिक अध्ययन ने यह भी संकेत दिया कि आई.टी.जेड. में फ्लाई ऐश कणों की बढ़ती उपस्थिति से पेस्ट की तुलना में मोर्टार के लचीलेपन में सुधार होता है। यह देखा गया था कि सीमेंट जल योजन मॉडल का उपयोग करके एक संगणन खंड में बड़े कणों के आसपास आई.टी.जेड. की सूक्ष्म संरचना का अनुकरण किया जा सकता है। मॉडलिंग अध्ययनों से पता चला है कि आई.टी.जेड. की सूक्ष्म संरचना के अंदर की विषमताएँ कंक्रीट की मज़बूती का नियंत्रण करती हैं। लचीलेपन पर प्रभाव की तुलना में

परिवहन गुणों पर इसका प्रभाव अधिक पाया गया। मॉडलिंग अध्ययन ने यह भी समझ आया कि आम तौर पर आई.टी.जेड. के प्रभाव को समझने के लिए किए गए प्रयोगात्मक अध्ययन कंक्रीट के समग्र व्यवहार पर आई.टी.जेड. के प्रभाव को क्यों नहीं दिखाते। मॉडलिंग के परिणाम मज़बूती के विकास पर फ्लाई ऐश के प्रभाव की अंतर्दृष्टि प्रदान करते हैं। यह देखा गया कि फ्लाई ऐश की पॉज़ोलैनिक प्रतिक्रिया से सी-एस-एच फोम में सी-एस-एच सामग्री में वृद्धि होती है। विशेषतः इसका प्रभाव आई.टी.जेड. में होता है जो कि फ्लाई ऐश मार्टर में ज़्यादा सरंध्रता होने के बावजूद उसकी मज़बूती को बढ़ता है। यह भी देखा गया कि सी-एस-एच की संरचना में परिवर्तन, जो आमतौर पर प्रयोगात्मक रूप से देखा जाता है, रासायनिक संरचना को प्रभावित कर सकता है लेकिन मोर्टार के लचीलेपन पर इसका प्रभाव बहुत कम होता है।

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Glossary

A	Al_2O_3
A/S	Alumina to silica ratio in C-S-H
AFm	Al_2O_3 - Fe_2O_3 – Mono
AFt	Al_2O_3 – Fe_2O_3 – Tri
BCP	Bulk cement paste
BSE	Back scattered electron
C	CaO
C/S	Calcium to silica ratio in C-S-H
C_3S	Alite or $3CaO.SiO_2$
C_2S	Belite or $2CaO.SiO_2$
C_3A	Aluminate or $3CaO.\ Al_2O_3$
C_4AF	Ferrite or $4CaO.\ Al_2O_{3.}\ Fe_2O_3$
$C\overline{S}H_2$	Gypsum
CH	Portlandite or $Ca(OH)_2$
C-S-H	Calcium silicate hydrate
DoH	Degree of hydration
EDX	Energy Dispersive X-Ray Spectroscopy
F	Fe_2O_3
H	H_2O
H/S	Molar ratio of water to silica in C-S-H
ITZ	Interfacial transition zone
OPC	Ordinary Portland cement
PSD	Particle size distribution
MIP	Mercury intrusion porosimetry
S	SiO_2
SCM	Supplementary cementitious material
SCS	Self-consistent scheme
SEM	Scanning electron microscopy
TGA	Thermogravimetric analysis
XRD	X-ray diffraction
XRF	X-ray fluorescence

Notation

$\boldsymbol{C}$	Localisation tensor that relates strain in the inhomogeneity to the strain in the C-S-H foam at level 1 of homogenization
$\ddot{\boldsymbol{C}}$	Localisation tensor that relates concentration gradient in the inhomogeneity to the concentration gradient in the C-S-H foam at level 1 of homogenization
$\boldsymbol{D}$	Diffusion tensor
$\boldsymbol{G}$	Localization tensor that relates strain in the inhomogeneity to the strain in the matrix
$\ddot{\boldsymbol{G}}$	Localization tensor that relates concentration gradient in the inhomogeneity to the concentration gradient in the matrix material
$\boldsymbol{I}$	Fourth order unit tensor
$\boldsymbol{L}$	Stiffness tensor
$\boldsymbol{O}$	Localisation tensor that relates strain in the inhomogeneity to the strain experienced by the C-S-H foam at level 1a of homogenization
$\ddot{\boldsymbol{O}}$	Localisation tensor that relates concentration gradient in the inhomogeneity to the concentration gradient experienced by the C-S-H foam at level 1a of homogenization
$\boldsymbol{P}$	Eshelby's tensor for concentration gradient
$\boldsymbol{T}$	Localization tensor that relates strain in the inhomogeneity to the applied strain
$\ddot{\boldsymbol{T}}$	Localization tensor that relates concentration gradient in the inhomogeneity to the applied concentration gradient
$\boldsymbol{S}$	Eshelby's tensor for strain
D_i	Diffusion coefficient of $(i)^{th}$ phase
$\overline{D}_{in}$	Diffusion coefficient of equivalent homogeneous sphere
D^{RVE}	Diffusion coefficient of representative volume element
$\overline{D}$	Effective diffusion coefficient of composite material
G_h	Hydrostatic coefficient of $\boldsymbol{G}$
G_d	Deviatoric coefficient of $\boldsymbol{G}$
$\ddot{G}_h$	Hydrostatic coefficient of $\ddot{\boldsymbol{G}}$
$\ddot{G}_d$	Deviatoric coefficient of $\ddot{\boldsymbol{G}}$
I_h	Hydrostatic coefficient of $\boldsymbol{I}$
I_d	Hydrostatic coefficient of $\boldsymbol{I}$
K_i	Bulk modulus of $(i)^{th}$ phase
$\overline{K}_{in}$	Bulk modulus of equivalent homogeneous sphere
K^{RVE}	Effective bulk modulus of representative volume element
$\overline{K}$	Effective bulk modulus of composite material
T_h	Hydrostatic coefficient of $\boldsymbol{T}$
T_d	Deviatoric coefficient of $\boldsymbol{T}$

$\ddot{T}_h$	Hydrostatic coefficient of $\ddot{\boldsymbol{T}}$
$\ddot{T}_d$	Deviatoric coefficient of $\ddot{\boldsymbol{T}}$
U	Strain energy stored
υ_{CSH}	Volume fraction of C-S-H gel in C-S-H foam
υ_p	Volume fraction of capillary pores in C-S-H foam
$\ddot{c}$	Ionic concentration
j	Ionic flux
ν_i	Poisson's ratio of $(i)^{th}$ phase
μ_i	Shear modulus of $(i)^{th}$ phase
$\bar{\mu}_{in}$	Shear modulus of equivalent homogeneous sphere
μ^{RVE}	Effective shear modulus of representative volume element
$\bar{\mu}$	Effective shear modulus of composite material
υ_i	Volume fraction of $(i)^{th}$ phase within the corresponding multi-coated inhomogeneity
η_y	Volume fraction of $(y)^{th}$ equivalent homogeneous sphere in the composite
σ_h	Trace of Cauchy's stress tensor
ε_h	Trace of strain tensor
$\alpha^{(\infty)}$	Applied concentration gradient at the boundary
$\boldsymbol{\sigma}$	Cauchy's stress tensor
$\boldsymbol{\varepsilon}$	Strain tensor
$\boldsymbol{\sigma_h}$	Hydrostatic part of Cauchy's stress tensor
$\boldsymbol{\sigma_d}$	Deviatoric part of Cauchy's stress tensor
$\boldsymbol{\varepsilon_h}$	Hydrostatic part of strain tensor
$\boldsymbol{\varepsilon_d}$	Deviatoric part of strain tensor
$\boldsymbol{\varepsilon}^{(\infty)}$	Applied uniform strain tensor at the boundary
$\bar{\boldsymbol{\varepsilon}}^{(0)}$	Average strain tensor in the matrix
$\mathbb{I}$	Second order unit tensor
$\mathbb{J}_2$	Second invariant of the deviatoric stress tensor