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# Multi-chemo physical approach to life-cycle assessment of structural concrete and soil foundation

# Abordagem multi-químico física para a avaliação do ciclo de vida de concreto estrutural e fundação em solo

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## Abstract

Coupled analysis of mass transport and damage mechanics associated with steel corrosion and ASR is presented for structural performance assessment of reinforced concrete. Multi-scale modeling of micro-pore formation and transport phenomena of moisture and ions are mutually linked for predicting the corrosion of reinforcement and volumetric changes. The interaction of crack propagation with corroded gel migration is simulated. Two computer codes for multi-chemo physical simulation (*DuCOM*) and nonlinear dynamic mechanics of structural concrete (*COM3*) were combined. This computational system was verified by the laboratory scale experiments of damaged reinforced concrete members under static loads, and has been applied to safety and serviceability assessment of existing bridges. The coupled system is extended to soil foundation-underground water-reinforced concrete interaction of mechanics and mass transport.

***Keywords:*** multi-chemo physics, corrosion, cracking, mass transport, performance assessment, fatigue, soil foundation

## Resumo

Análise acoplada de transporte de massa e mecânica do dano associados com a corrosão do aço e RAS é apresentada para a avaliação do desempenho estrutural do concreto armado. Modelagem multi-escala da formação de micro-poros e fenômenos de transporte de umidade e íons são mutuamente interligados para prever a corrosão de armadura e mudanças de volume. A interação de propagação de fissuras com a migração de gel de corrosão é simulada. Dois códigos computacionais para a simulação multi-químico fisica (DuCOM) e dinâmica não-linear do concreto estrutural (COM3) foram combinados. Esse sistema computacional foi verificado por experimentos em escala laboratorial de elementos de concreto armado danificada sob cargas estáticas, e tem sido aplicado a segurança e avaliação em serviço de pontes existentes. O sistema acoplado é estendido à interação do comportamento mecânico e transporte de massa de fundação em solo, água subterrânea e concreto armado

***Palavras-chave:*** multi-químico física, corrosão, fissuração, transporte de massa, avaliação de desempenho, fundação em solo

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## 1 Introduction

In the scheme of performance-based design with more transparency to clients and taxpayers, performance assessment methods occupy a central position from a viewpoint of structural mechanics and engineering. This rational way of assuring the overall quality of infrastructures may create cost-beneficial design and construction that exactly satisfies several requirements assigned to engineers. Life-cycle performance of structures is being explicitly required, and appropriate design methods for materials and structures are sought in several societies and organizations. Furthermore, needs to verify remaining functionality of damaged existing facilities is rising for extending service life. To meet these challenges, keenly expected is an explicit prediction and simulation of structural life serviceability and safety under specified loads and ambient conditions.

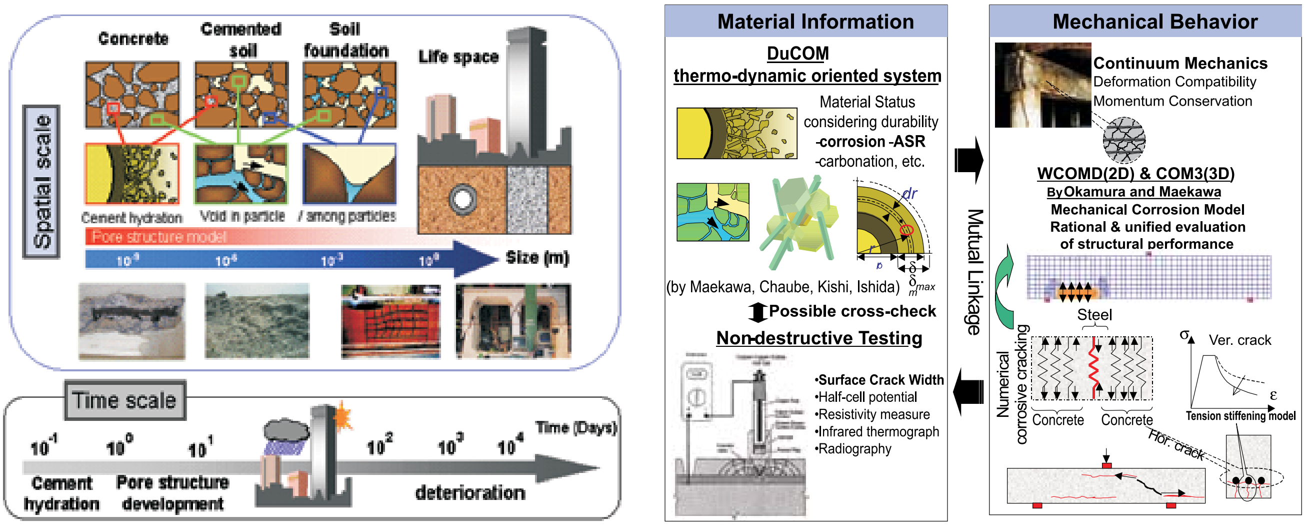
In this paper, the authors propose an integrated platform of solid mechanics and thermo-hydro dynamics of materials and structures with multi-scales of referential control volume on which each chemo-physics is applied. Inn more detail, the constitutive model is discussed with regard to cracking in RC elements, and overlay of thermo-hydro state variables is presented for multi-scale and multi-chemo mechanical coupling with soil foundation. Recent application of the multi-scale approach to practical problems is introduced, and the direction of future development is discussed as an integrated knowledge-base of structural concrete and soil foundation.

## 2 Multi-Directional crack mechanics

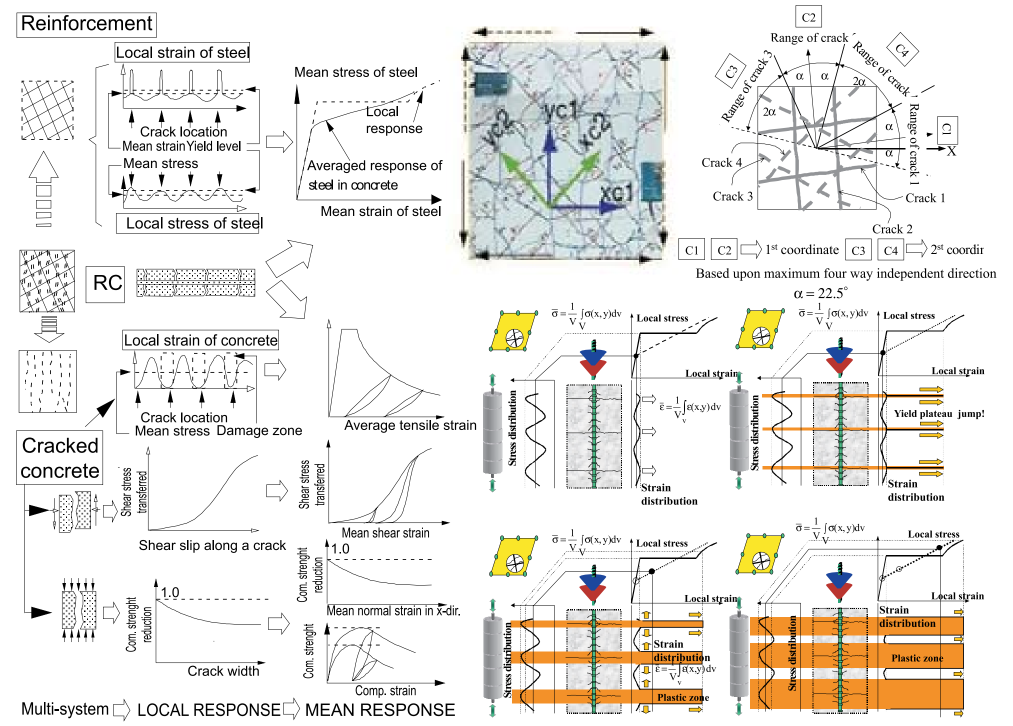
A scheme of RC modeling used for an integrated platform of both safety and life-cycle assessment is simply illustrated in Fig. 1 (Maekawa *et al*. 1999, 2001, 2003, Nakarai *et al.* 2005a, 2005b). Multi-directional cracking and its interaction are taken into account by the active crack approach (Maekawa *et al*. 2001) on the smeared compression stress field (Collins and Vecchio 1982). All microscopic physical states (cracking, yielding, crack shear slip, remaining stiffness of fractured materials) are included in the constitutive modeling. The stress carrying mechanisms are composed of compression/ tension parallel and normal to cracking and shear transfer. By the active crack method (Maekawa *et al*. 2001), the primary cracking of governing nonlinearity of structural concrete is identified if some cracks intersect non-orthogonally. Here, path-dependent parameters are renewed only along the active crack in each load step of time.

For seismic analyses in time domain, the plastic localization of reinforcement is of importance for rationally simulating largely deformed elements. The spatial averaging of local stress and strain along reinforcement is applied for structural analysis with finite elements as shown in Fig. 2. Since the local yield occurs at the crack location and the rest of domain generally remains elastic, the averaged stress strain relation of deformed reinforcing bars differs from that of a single bare bar. The following hardening of the element is much associated with extension of plastic zones and the averaged hardening stiffness is computed by considering the reinforcement ratio, tensile strength of concrete and properties of reinforcing bars (Maekawa *et al*. 2001). When the load reversal is produced in a single direction, near orthogonal two-way cracking is experienced. Here, the crack-to-crack mutual interaction is not so great as to consider the shear transfer of each intersecting cracks. Then, the smeared crack methods that assume coaxiality of stress and strain fields (rotating crack) may function successfully for structural analysis, and the model of shear transfer does not play a central role of mechanics.

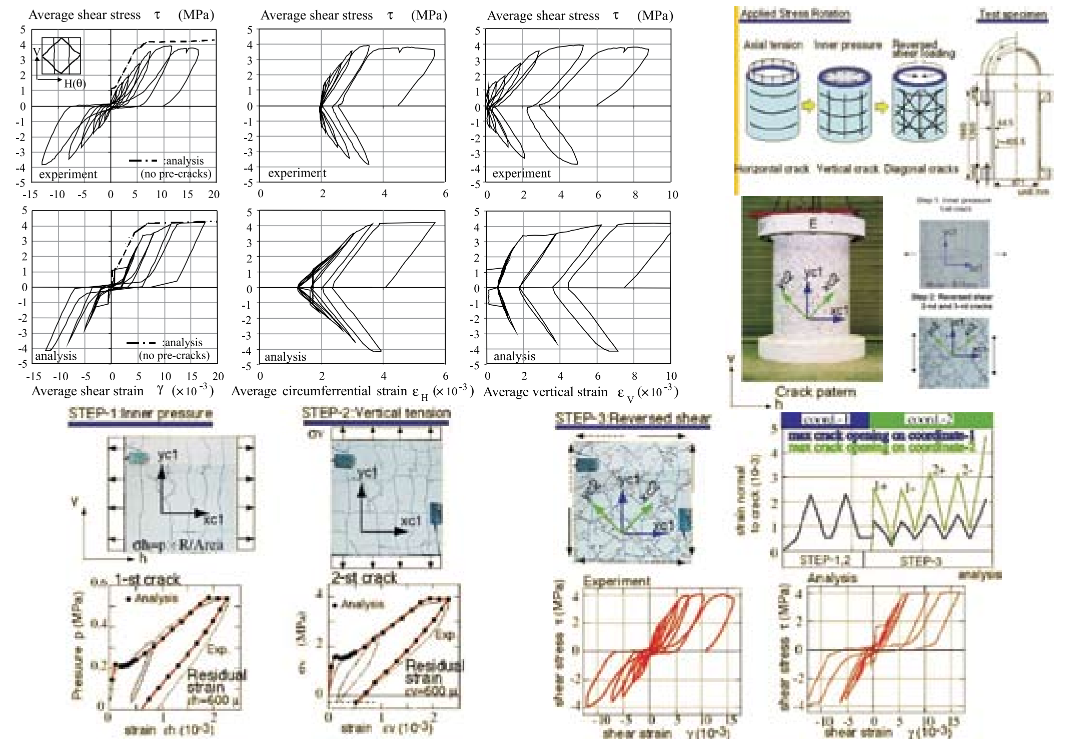
Figure 1 – Coupling of thermo-hydro dynamics and damage mechanics for life cycle assessment of structures with soil foundation interaction



### Figure 2 – Formulation of in-plane constitutive model with multi-directional cracking



### Figure 3 – Experimental and analytical behavior of specimens A-2 (4-way cracks)



However, the multi-directional and non-proportional loadings may create three and four directional cracking that intersects each other in finite element domain. When thermal and drying expansion and shrinkage would be coupled with seismic loads, principal stress directions considerably rotate. This situation tends to create multi-directionally intersecting cracking with strong interaction. Figure 3 shows an example of experimental verification with three and four directional cracking in two-way reinforced RC panels under combined in-plane shear and normal stresses. The in-plane stresses were actively controlled by the internal hydraulic pressure, torsion moment produced by a couple of jacks and axial compression. The non-orthogonal crack intersection frequently takes place when the principal direction of applied loads varies and/or external forces and ambient actions are coupled together. Constitutive models have to be verified on member/structural levels, because stress states and loading paths cannot be fully reproduced only by experiments at the specimen level under rather uniform fields of stress and strain. Shear wall experiments have been used for verification of in-plane RC modeling under monotonic as well as cyclic loads (Maekawa *et al*. 2001) of small numbers of repetitions. It is recognized that in-plane RC models are well applied under both static forces and dynamic excitation. The verification has been extended to 3D shells, beam-column lineal members and closed frames (tunnel model) surrounded by soil foundation. The inelastic creep and fatigue in compression, tension and shear transfer along crack planes have been included in the computational platform (El-Kashif *et al.* 2004).

Figure 4a shows the experimental verification by using the real scale mockup for tunnels and ducts. Here, the shear capacity and ductility were carefully focused on. The multi-directional cracking model has been examined as well by reproducing alternate change of principal stress directions in 3D spaces (See Figure 4b). For practical use of the computational platform, the multi-plastic potential model for soil skeleton is included with the underground pore water to take into account liquefaction. Figure 4c shows the soil container which includes the RC box culvert and was set on the shaking table. The soil pressure applied on the walls of the embedded RC duct and the average shear deformation of the structure was carefully compared with the analytical results. Right now, the nonlinear finite element analysis is authorized as a tool to examine the seismic safety performance in the scheme of designing LNG storage tanks and RC aquaducts for nuclear power plant facilities for practice in Japan.

Figure 4a – RC underground box-vents subjected to static loads. (Soraoka et al. 2001)

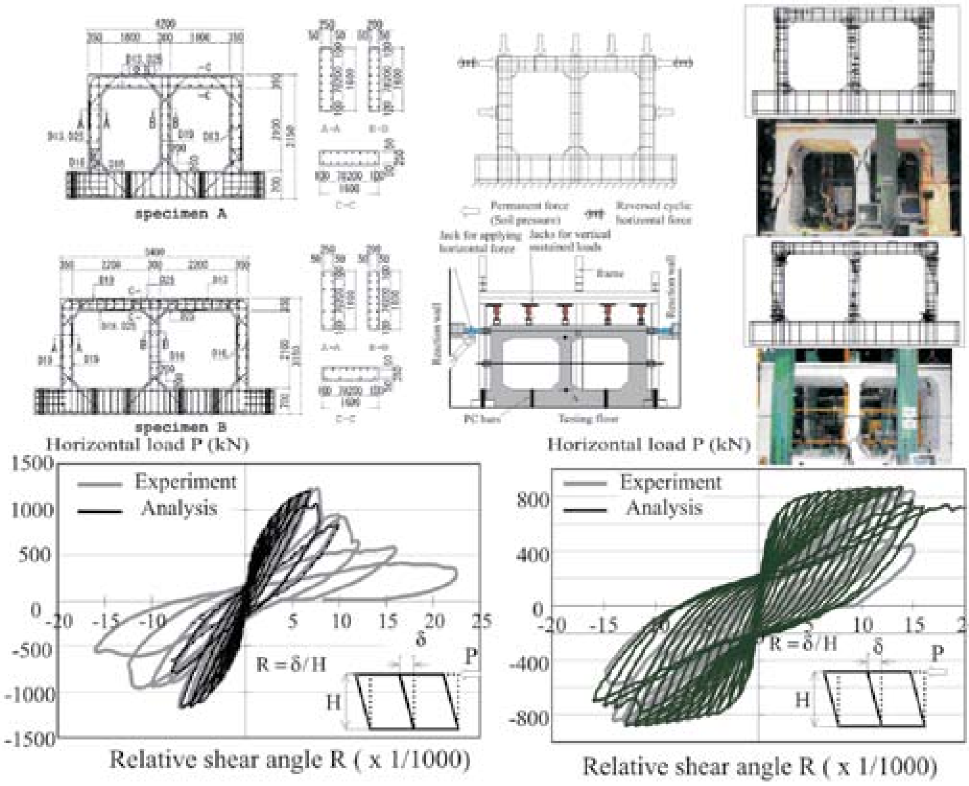


Figure 4b – RC structures subjected to multi-directional static loads

## 3 Thermo-hydro chemo-pysical modeling

State variables of thermo-hydro dynamics are further required for life-cycle assessment, especially for durability assessment related to material properties. Volumetric change caused by temperature and long-term moisture equilibrium in micro-pores are associated with cracking and corresponding serviceability, and corrosion of reinforcement has much to do with migration of chemicals through micro-pores. Thus, the coupled system as shown in Fig. 5 was proposed

(Maekawa *et al*. 1999, 2003) to simulate the entire thermo-mechanical states of constituent material and structures. For computing the thermo hydro equilibrium, multi-scale analysis platform *DuCOM* (Maekawa *et al*. 1999, 2003) was used. Micro-pore geometry and spaces are idealized by statically formulated pore distribution and internal moisture balance is simultaneously solved with mass conservation requirement. The moisture migration and diffusivity are computed based on the micro-pore size distribution and the space of condensed water channel.

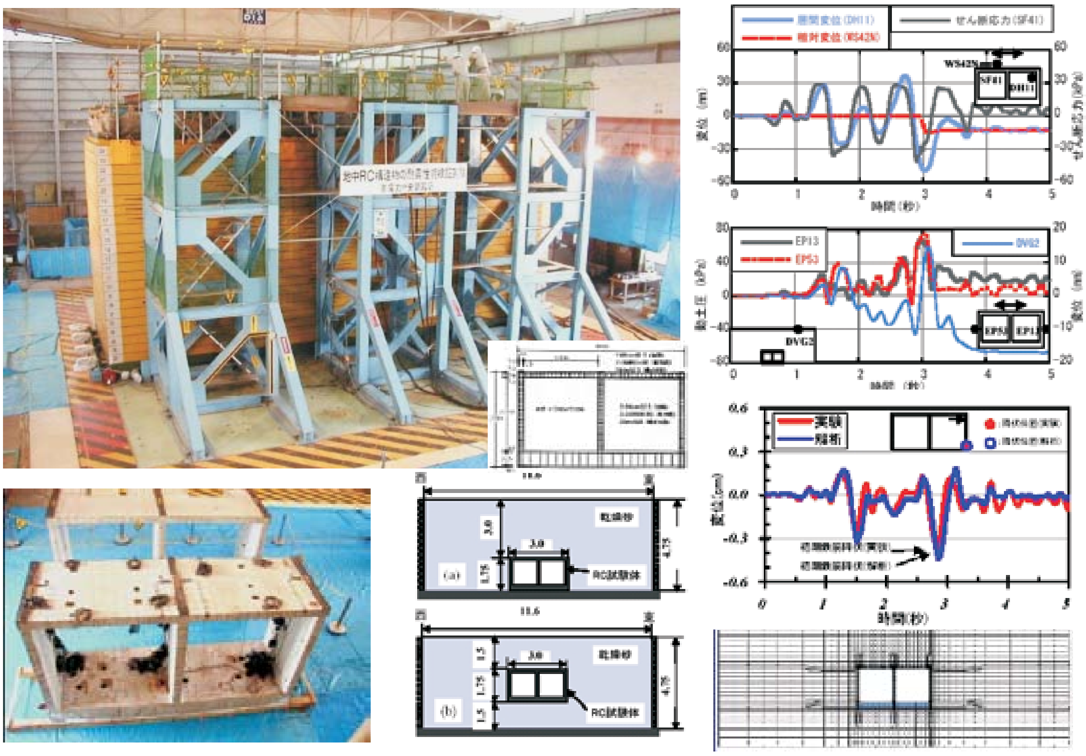
Chloride ion migration and other chemical reactions such as carbonation and calcium leaching are overlaid on this system (Maekawa *et al*. 2003, Nakarai *et al*. 2005a). The conductivity and diffusion characteristics for mass transport are calculated based upon computationally formed micro-pore structure. The computation of multi-chemo-physical events is carried out by means of the sequential processing with closed-loop predictor-corrector method (Fig. 5) (Maekawa *et al*. 2003). The temperature dependent volume change is considered as an offset strain in constitutive modeling. But, concrete shrinkage associated with microclimate in CSH gel and capillary pores is directly linked with the macroscopic constitutive model (see Section 2) with regard to micro-pore pressure and disjoining pressure originated from *Van del Waals* and *Coulomb* forces.

Micro-corrosion rate is also computed by simulating migration of $O_2$-$CO_2$ gas and chloride ion (Maekawa *et al*. 2003), and the effect of corrosion is integrated in the structural analysis (Toongoenthong and Maekawa 2005). These thermodynamic state variables are incorporated into the constitutive modeling before cracking. In this computation, the thermo-dynamic equilibrium requirements are simultaneously solved such as multi-ion balance, proton electro-balance, adsorption-desorption isotherm (see Fig. 5). Then, we have approximately 230 simutaneous equations to be solved numerically for chemo-physical and mechanical behaviors of different scales.

(a) Statistical expression of CSH micro-porosity and the moisture equilibrium under pore moisture potential.

(b) Flowchart of solving multi-chemo physical events

Figure 4c – RC underground box-vents subjected to dynamic shear (JSCE, 1999)

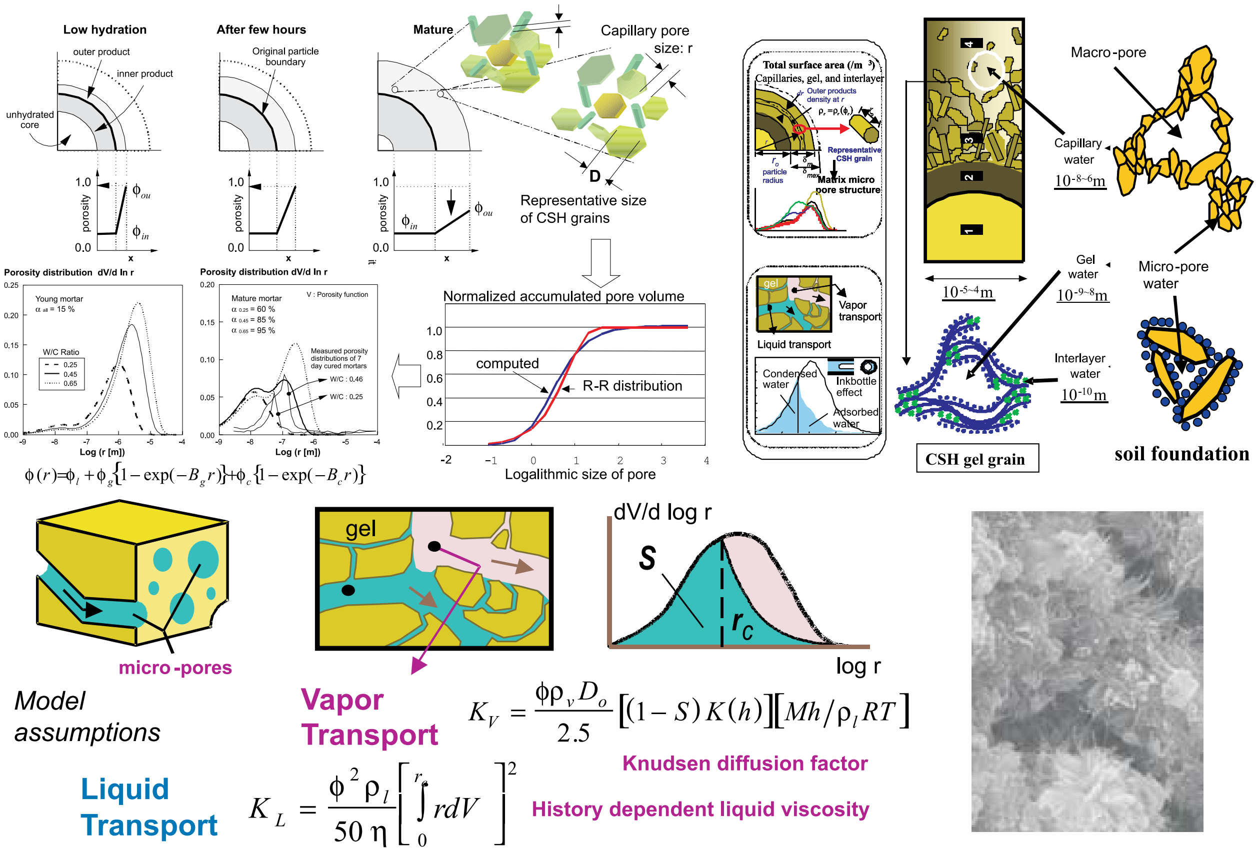


## 4 Coupling of damage mechanics with chemo-pyiscal events

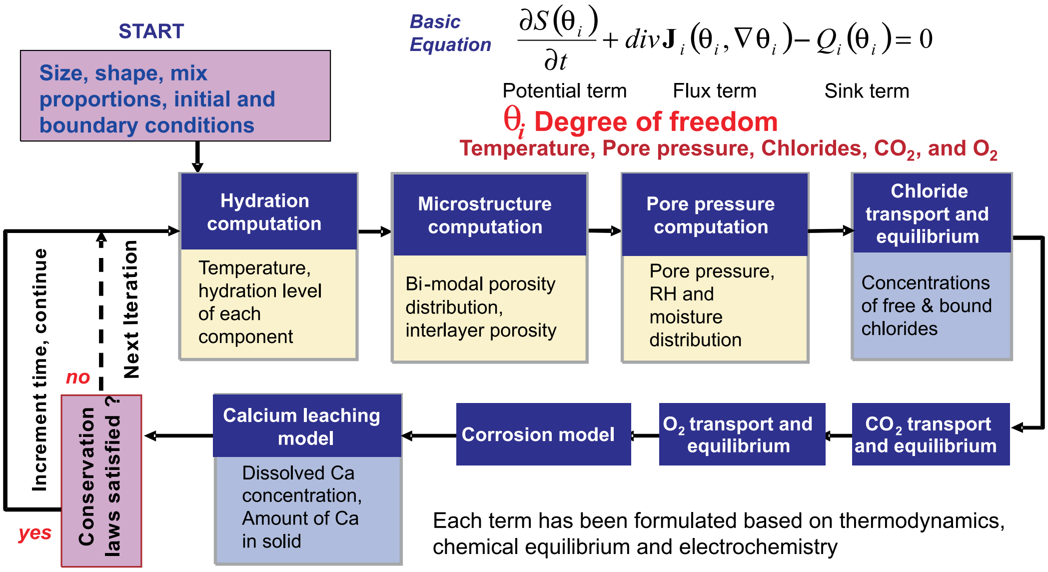
Cracking is also influential in mass transport of gases and dissolved ions. These cracks through which ion substances can easily migrate are mutually linked with thermo-hydro dynamic analysis by the hierarchy type of multi-scale modeling as shown in Fig. 5. This simulation can be mainly used for life-cycle assessment of structural concrete and examination of remaining functions of existing infrastructures. Cracking of concrete causes accelerated diffusion of chloride. It may allow deeper penetration of chloride and other substances. In the analysis, diffusivity of substances is regarded as a variable in terms of computed averaged strain of concrete finite elements.

The corroded steel produces volumetric expansion and results in internal self-equilibrated stress, which may lead to additional cracking around reinforcing bars. Figure 6 illustrates the way to amalgamate the damage mechanics and volume expansion of generated corrosion gels. The effect of corrosion gel product formation is considered in the constitutive modeling of reinforcement in the transverse direction. The non-corroded core steel and the corroded clusters with different mechanical properties are treated as a fictitious aging material of varying volumetric stiffness and expansion according to the magnitude of corrosion. This growing steel is em-

## Figure 5 – Micro-modeling of CSH gel and capillary pores and multi-chemo physics

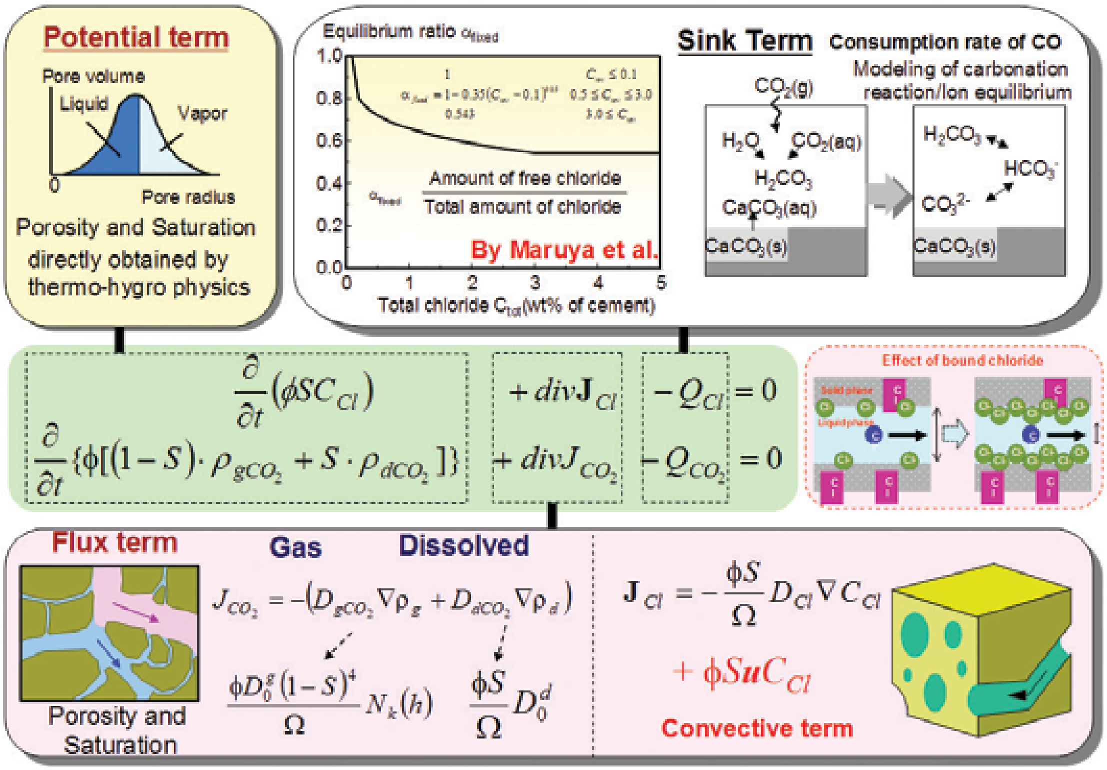


(a) Statistical expression of CSH micro-porosity and the moisture equilibrium under pore moisture potential



(b) Flowchart of solving multi-chemo physical events

**Figure 5a – Micro-modeling of CSH gel and capillary pores and multi-chemo physics**



bedded in each finite element similar to smeared crack approach as well.

If the corrosion is concentrated around the anchorage zone of main reinforcement, its structural capacity gets reduced with the different crack propagation pattern from those of sound ones (Toongoenthong and Maekawa 2004a, 2004b) (see Fig. 7). The diagonal crack which reaches the bending compression zone is initiated by the corrosion crack tip created along the longitudinal main reinforcement. Finally, the diagonal crack is driven to the beam support. Apparently, the localized corrosion is seen to deteriorate the anchorage performance of longitudinal reinforcement. The acceleration test of corrosion of steel in RC beam by galvanostatic charge also substantiated this simulation result.

When the corrosion cracking develops over the beam, shear safety performance differs from the non-damaged reference case (Satoh *et al*. 2003). Figure 7b shows load-displacement relations for RC non-damaged reference and corroded specimen, which was submerged into a sodium pond for accelerated corrosion. Here produced was uniformly distributed corrosion along the whole longitudinal steel of 2.1% as the mass loss.

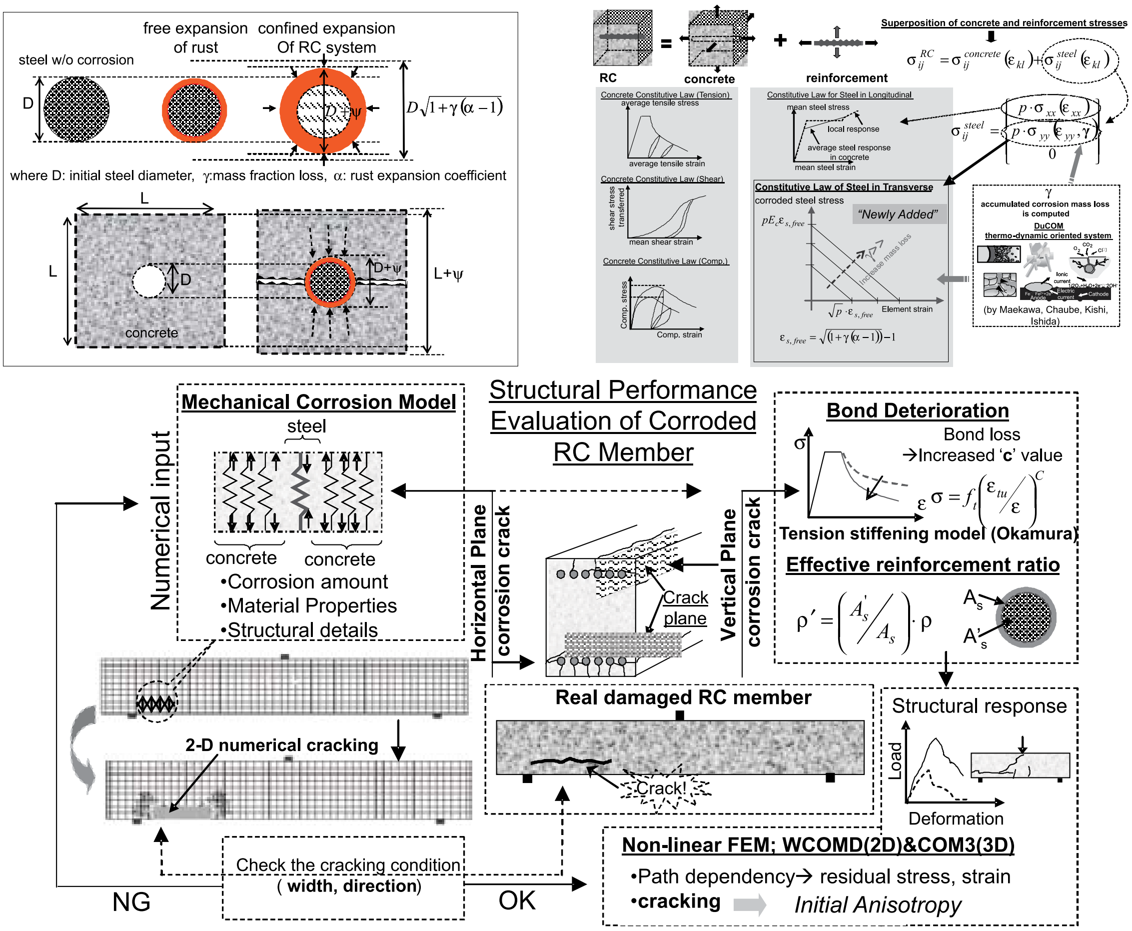
Main reinforcing bars were bent up 90 degree inside the anchorage zone**.** Thus, comparatively satisfactory anchorage capacity is expected. In this case, the stiffness of the beam is much reduced but the capacity is a bit increased. The macroscopic bond loss in the shear span leads to retarded propagation of diagonal shear cracking and may elevate the shear capacity. Computation can capture this property.

Figure 8 shows the corrosion crack propagation in experiment and simulation. The corrosive mass loss can be computed by *DuCOM* under the constant chloride concentration on the surface (see section 3). The corrosion gel product is assumed to be created around the mother steel bars and the transverse stress normal to the reinforcement axis is computed as shown in Figure 6. The crack patterns of the same surface crack width and the corresponding corrosion mass loss are compared with each other. The crack orientation and ligaments are fairly simulated. In these analyses, the injection of corrosion products in colloidal gels into crack gaps was taken into account in the analysis. Otherwise, the rational simulation of corrosion cracking and the life of concrete cover may not be earned.

Figure 9 shows the fatigue simulation of RC beams under high cycle shear. If the pre-corrosion crack develops around the anchorage zone of the web reinforced beam, the fatigue life is tremendously degraded even though the static capacity is almost the same as that of the non-damaged one.

On the contrary, the pre-corroded cracking inside the shear span brings much longer fatigue life to non-web reinforced members due to the loss of macroscopic bond. The corroded cracks along main reinforcement results in arch-action formed between the supports and the loading point against

**Figure 6 – Simulation of corrosion of r/f bars and structural performance assessment**



shear. This fact was experimentally verified too in use of actually damaged RC slabs for railway infrastructures.

Autogenous and drying shrinkage, which is computed by solving the moisture migration under ambient conditions (Mabrouk *et al*. 2004), can be directly included in the constitutive modeling of concrete in each finite element as shown in Fig. 10. The coupling of concrete creep in compression, shrinkage and post-cracking time-dependent tension stiffness models yields consistent behavioral simulation with reasonable accuracy for long-term deflection.

Figure 11 shows the application examples for the seismic performance assessment of underground LNG storage tanks, existing bridge piers in service and urban in-ground and underground transportation infrastructures in the capital city of Tokyo. Multi-chemo-mechanistic nonlinear finite element analyses bring about high cost performance and behavioral simulation of structures of geometrical complexity with soil interaction.

Figure 12 is the recent example of application to the engineering assessment for a 100-years old railway bridge in Tokyo (Sogano *et al*. 2001). Due to uneven settlement of the foundation, some initial damage remains in the form of cracking and arch ribs were strengthened by additional RC arch inside layer in the past. The seismic ground motion was applied to the numerically aged structural concrete and the computed response was used for safety and serviceability assessment in practice. The seismic remaining performance was numerically investigated and the sustainable life with light retrofit was judged.

Figure 13 shows the analysis for remaining structural safety of ASR damaged RC bridge piers. As lots of reinforcing bars are ruptured at the inside corners of bent portions, anchorage performance of web reinforcement is thought to be deteriorated. But, as a matter of fact, the capacity of ASR damaged members was predicted to increase in accordance with magnitude of ASR expansion. This is attributed to the pre-stressing effect and self-equilibrated compressive axial force. After the peak of capacity, it starts to decline. Thus, the way of strengthening and/or repair must be different according to the induced expansion.

Figure 14 shows the PRC bridge in which plenty of cracks

**Figure 7a – Analysis result of beam with inherent crack-like defect till the anchorage zone**

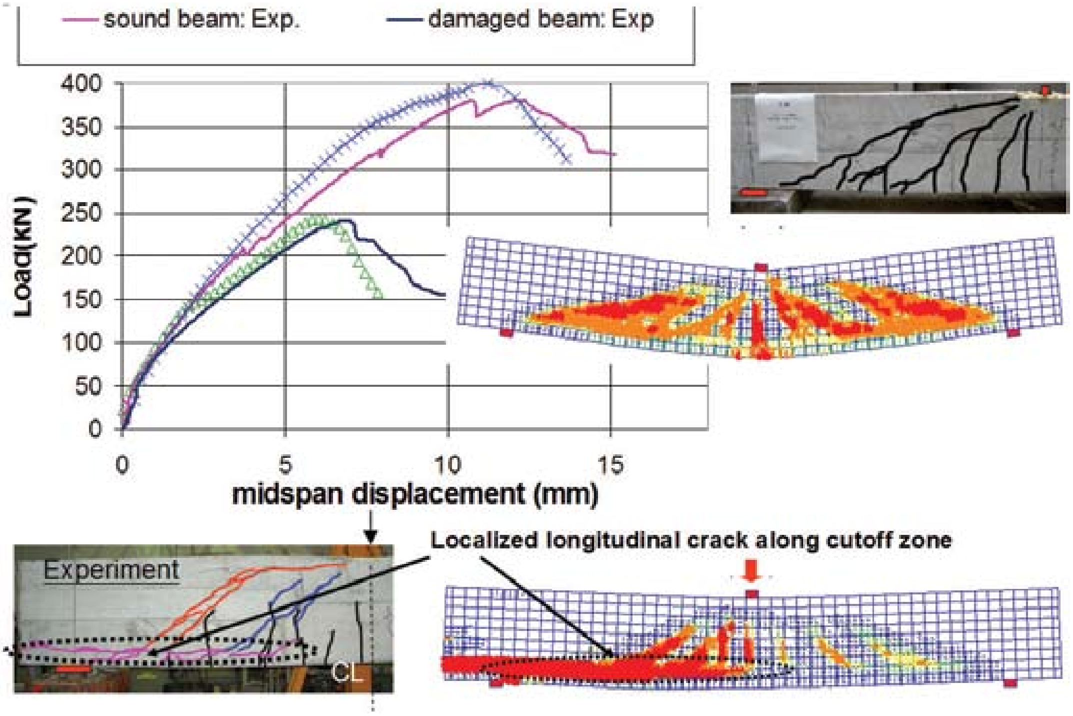
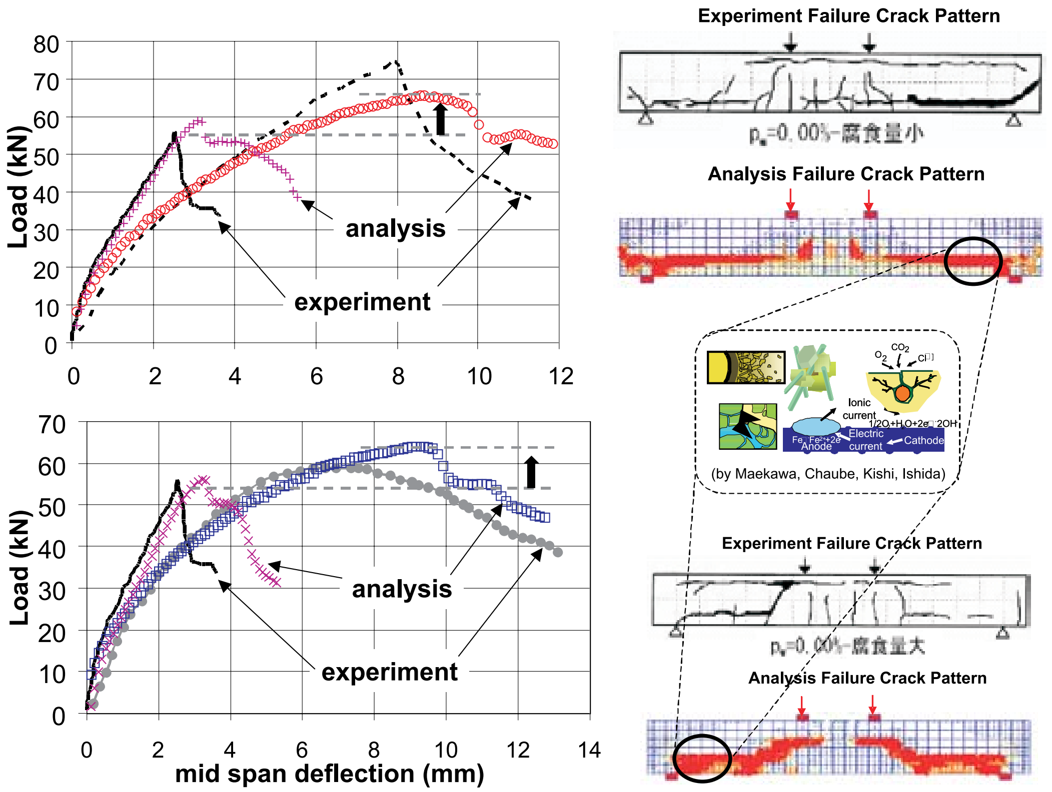


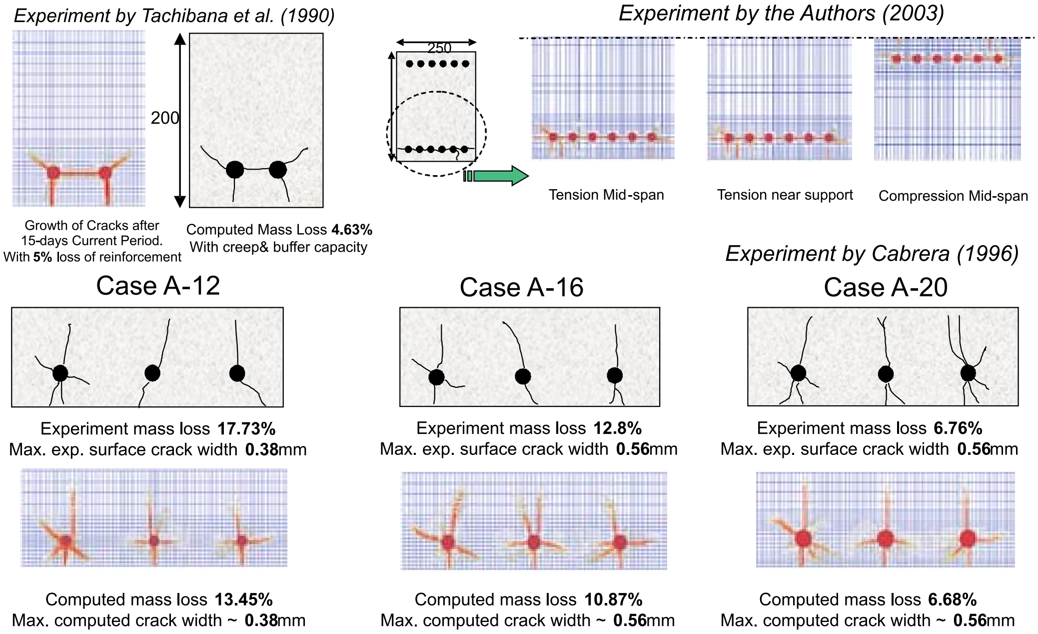
**Figure 7b – Simulated shear capacity and cracking of corrosion beam**



a) Load-displacement relation

b) Failure crack pattern

**Figure 8 – Simulated shear capacity and cracking of corrosion beam (Toongoenthong and Maekawa 2005)**



were induced to the viaducts due to excessive shrinkage of concrete and heavy reinforcement. The compliance of the viaduct in each span was reported to be much increased and the fatigue life was questioned. JSCE concrete committee (2005) investigated the detailed damage and corresponding remaining fatigue life by using the coupled chemo-mechanical simulation. For verification of the analysis method, the design live load (150 tonf) was applied on the deck and the incremental deflection was measured as shown in Fig. 14. The simulation was reported to be closer to the reality of the damaged PRC bridge.

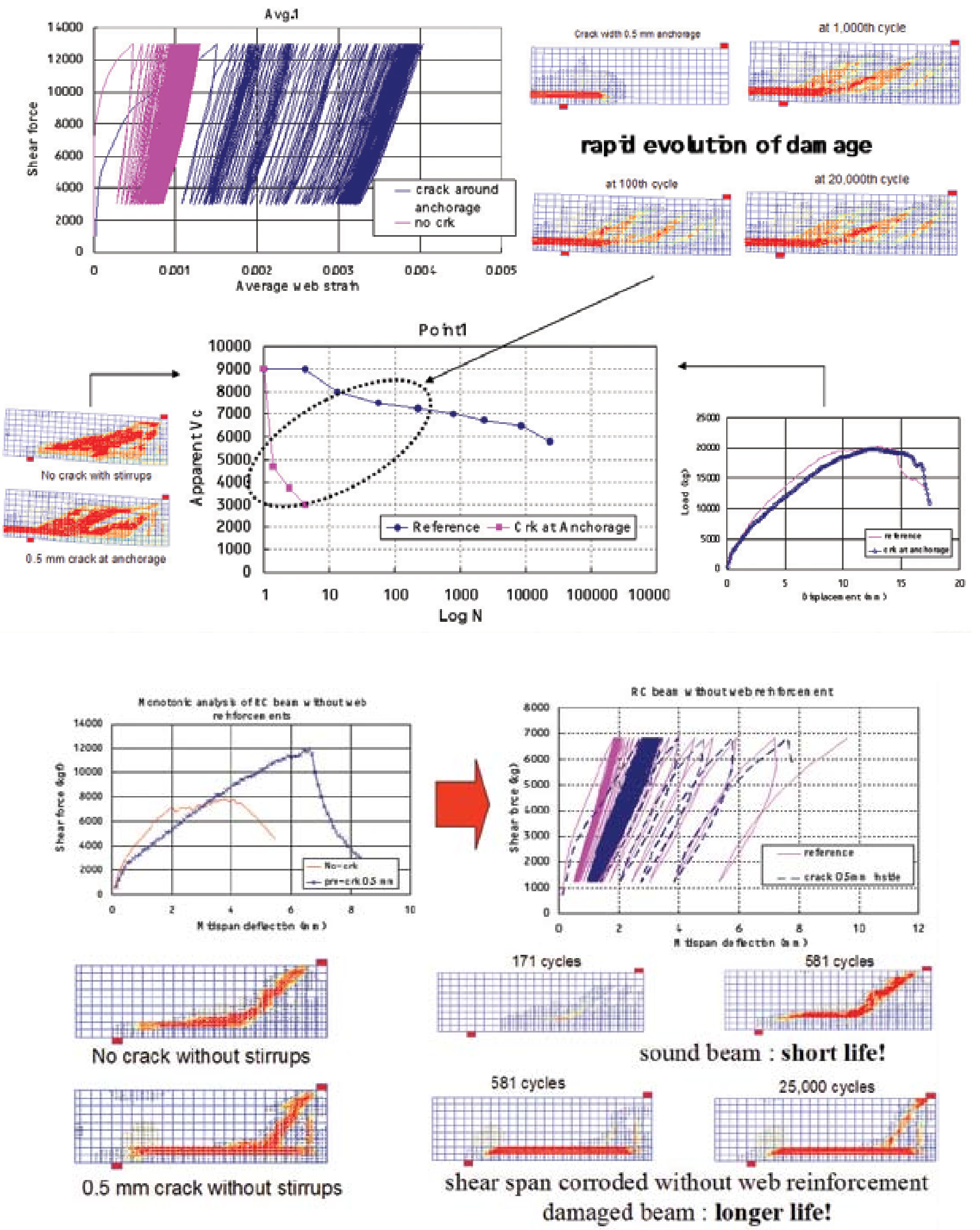
## 5 Coupling with soil foundation system

The multi-scale modeling of cementitious composites can be extended to soil foundation with large-scale pores of strong connectivity. Figure 15 summarizes the micro-pore distribution modeling and the mass transport modeling through micro-pores was extended to the large-scale pores among soil grains (Nakarai *et al*. 2005b). Verification was conducted in use of experimentally obtained permeability. Leaching and mass transport of calcium ion were mounted on this extended system for estimating extremely long-term performance of underground concrete structures and environmental issues of underground water. This extended simulation method can also treat the life-cycle assessment of cementitious soil. Figure 16 shows analytical and experimental results of calcium leaching from the cemented sand. Leaching is associated with permeability and bulk motion of water, whose characteristic is greatly influenced by the micro-pore structure. This is not a given material constant but computed value in the multi-physicochemical scheme.

Figure 17 shows an analysis and verification of calcium leaching from underground concrete structures into the soil environment. Different boundary conditions are assumed; exposed to water with constant concentration and soil foundation with no bulk motion of underground water. The degree of deterioration obtained from the coupled analysis is much lower and closer to the measurement results than the results of the analysis that did not include the surrounding ground. The results indicate that the interaction with soil foundation is critical for assessment of leaching of underground structure (Fig. 14).

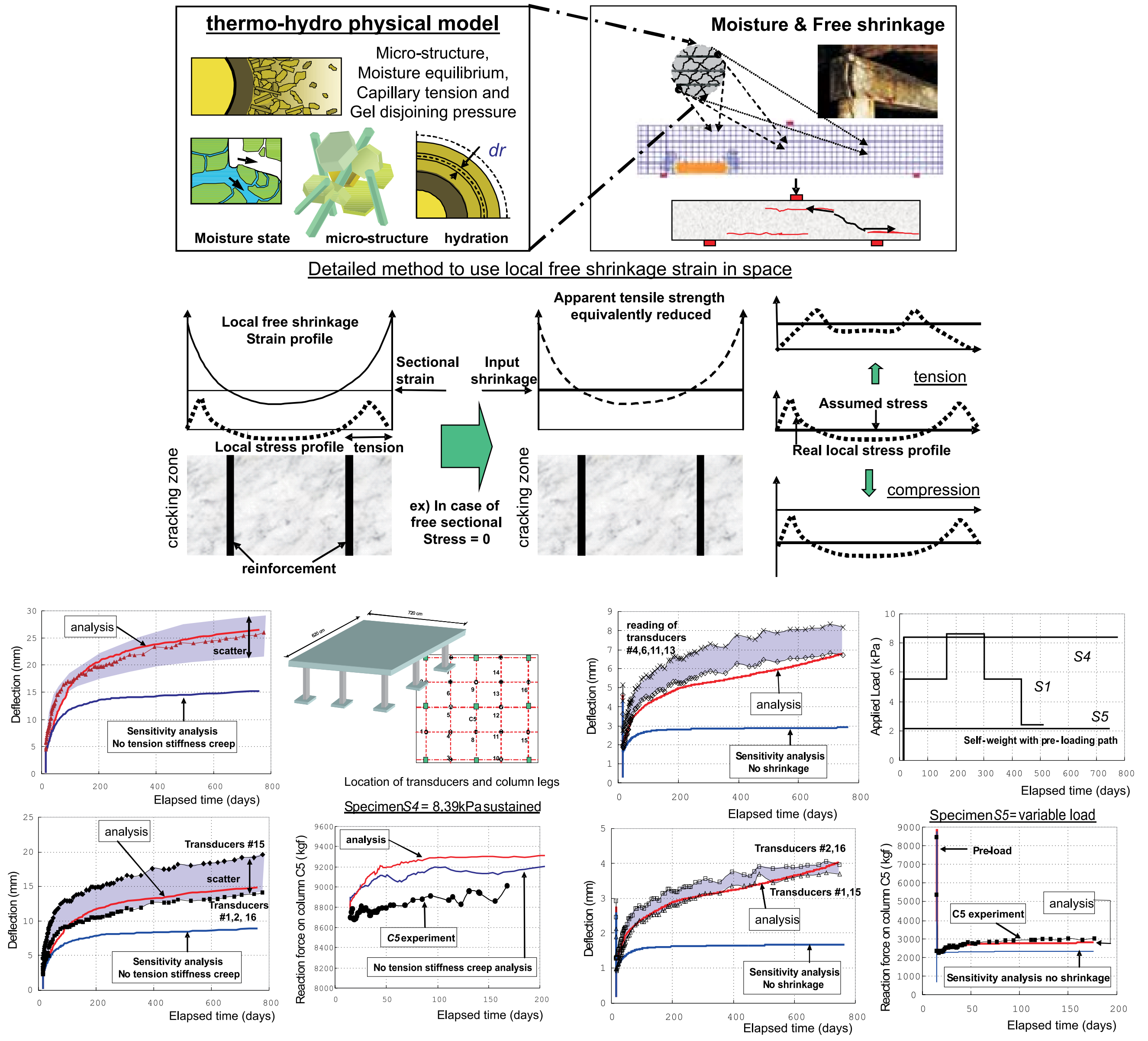
Figure 18 describes the outline of the modeling for calcium ion behavior in the bentonite in order to investigate the influence of surrounding bentonite on the concrete barrier. The model consists of the calcium liquid-bound equilibrium model and the calcium ion transport model. The equilibrium model treats the binding of the calcium ion caused by the dislocation of sodium ions in montmorillonite and the calcium ion electrically absorbed on the surface of the bentonite as bound calcium ion. The relation between bound and liquid calcium was determined based on the results of a simplified experiment in which bentonite particle was soaked in calcium oxide solution. In the ion transport model, the constrictivity is taken into account as a reduction parameter for diffusivity. The constrictivity was defined as a function of thickness of montmorillonite layer based on the experiments of Sato *et al*. (1995). The thickness can be obtained

**Figure 9 – Simulated shear capacity and cracking of corrosion beam under fatigue loads**



from the dry density and properties of bentonite based on the equation proposed by Komine and Ogata (1999). Figure 19 shows analytical results that investigate the effect of the surrounding bentonite on the long-term calcium leaching from concrete (Nakarai *et al*. 2005a). The results imply the possibility of accelerated leaching by the sur-

**Figure 10 – Simulated shear capacity and cracking of corrosion beam under fatigue loads (experiment by Guo and Gilbert, 2002)**



rounding bentonite. This is because a low concentration of free calcium ions in the pores of the surrounding bentonite was maintained due to the high binding capacity of ions and the constantly high concentration gradient between the concrete and the bentonite.

## 6 Conclusions

Chemo-physical and mechanical modeling of concrete with greatly different scales of geometry was presented, and synthesized on a unified computational platform, which may bring about quantitative assessment of structural concrete performances of interaction with soil foundation. The safety assessment method was extended to the life-cycle issue with multi-scaled information on microclimate states of cementitious composites under macroscopic ambient boundary conditions. Currently granted is a great deal of knowledge earned by the past development. At the same time, we face a difficulty to quantitatively extract consequential figures from them. The authors expect that the systematic framework on the knowledge-based technology will be extended efficiently and can be steadily taken over by engineers in charge.

The authors' appreciation is addressed to Dr. Kishi for valuable discussion. This study was financially supported by Grant-in-Aid for Scientific Research (S) No.15106008.

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Figure 11 – Safety assessment of transportation infrastructures against earthquake

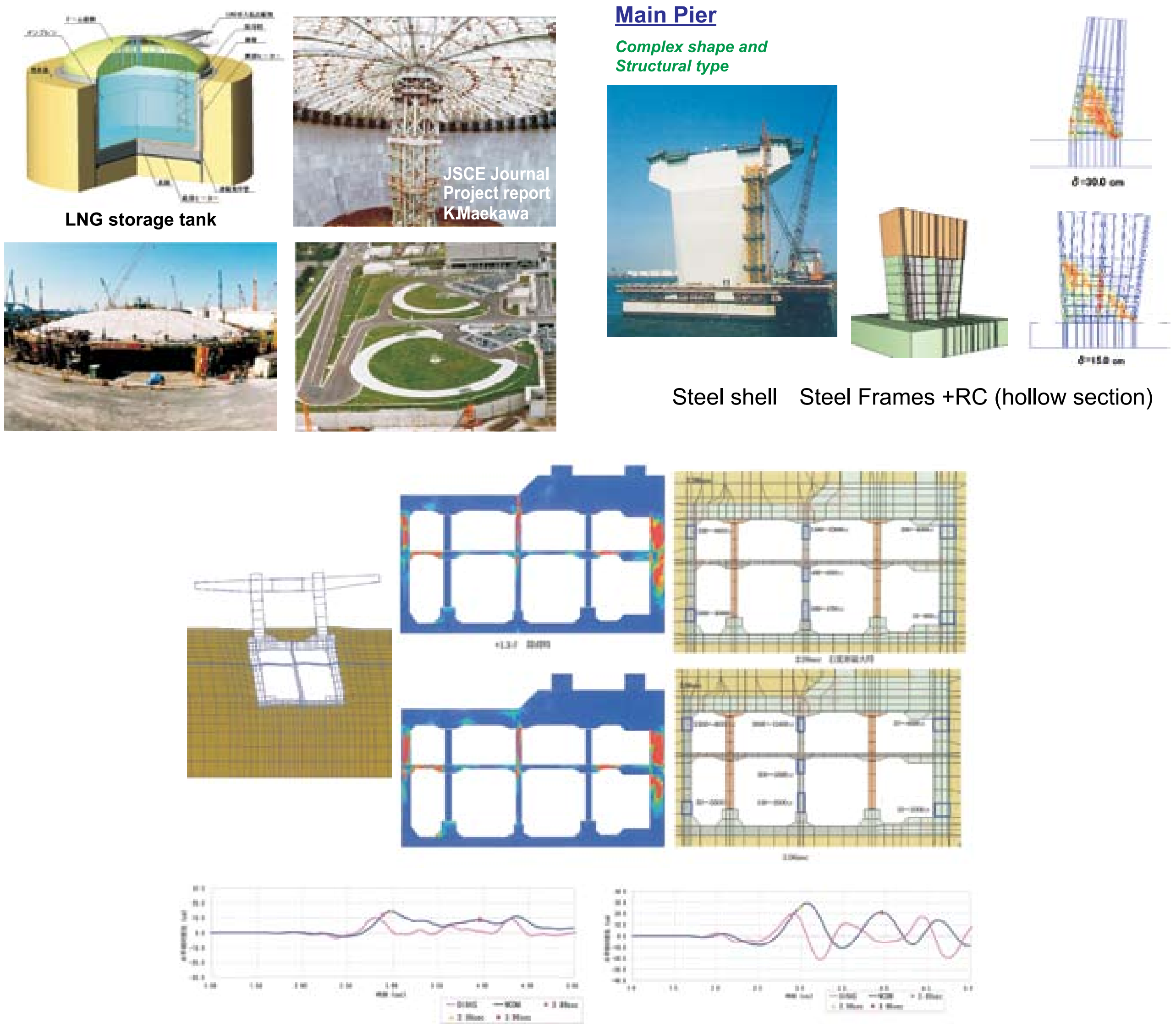


Figure 12 – Safety assessment of 100 years-old railway bridges (Sogano et al. 2001)

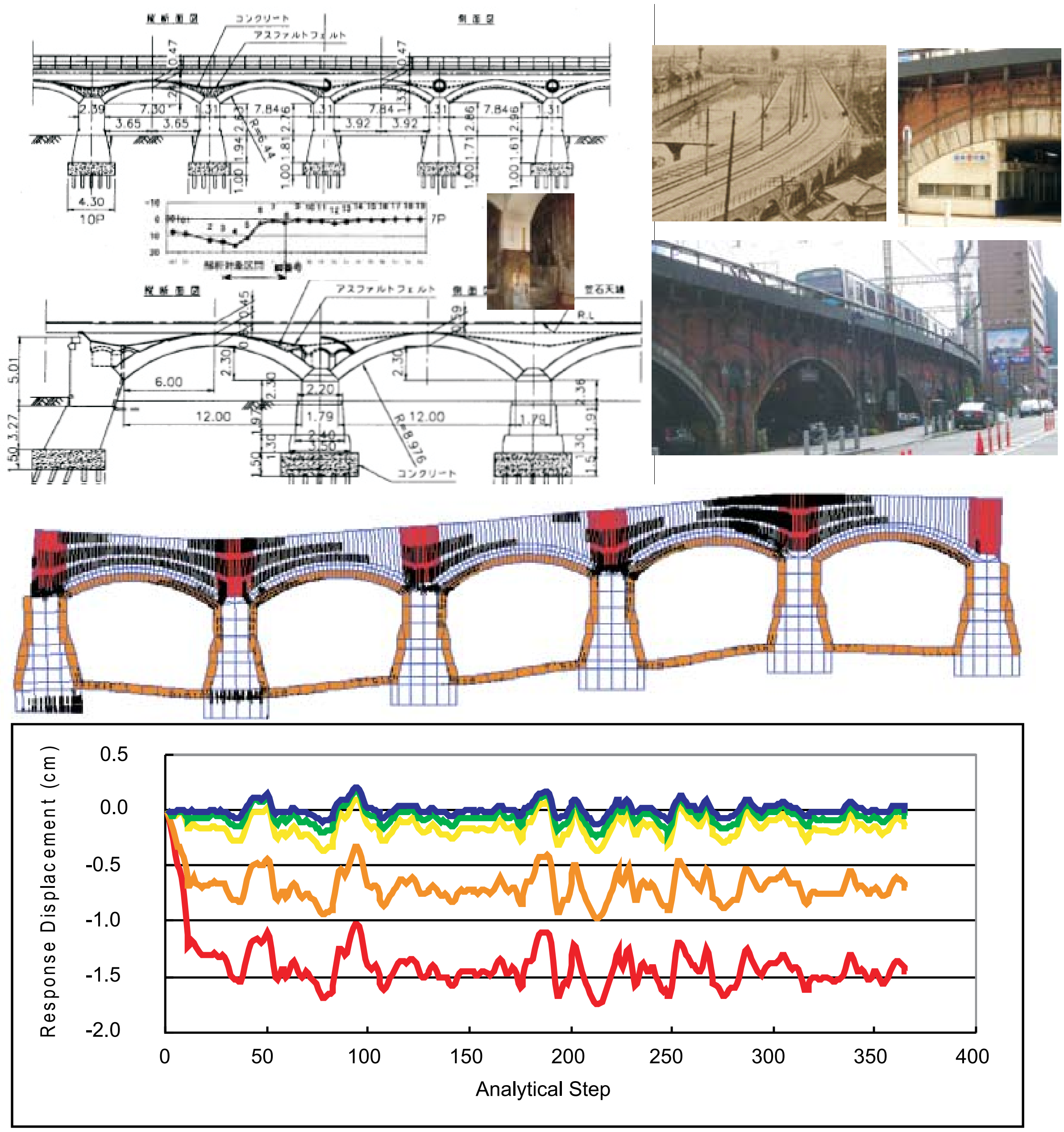


**Figure 13 – ASR damaged RC bridge pier and capacity simulation (JSCE, 2005)**

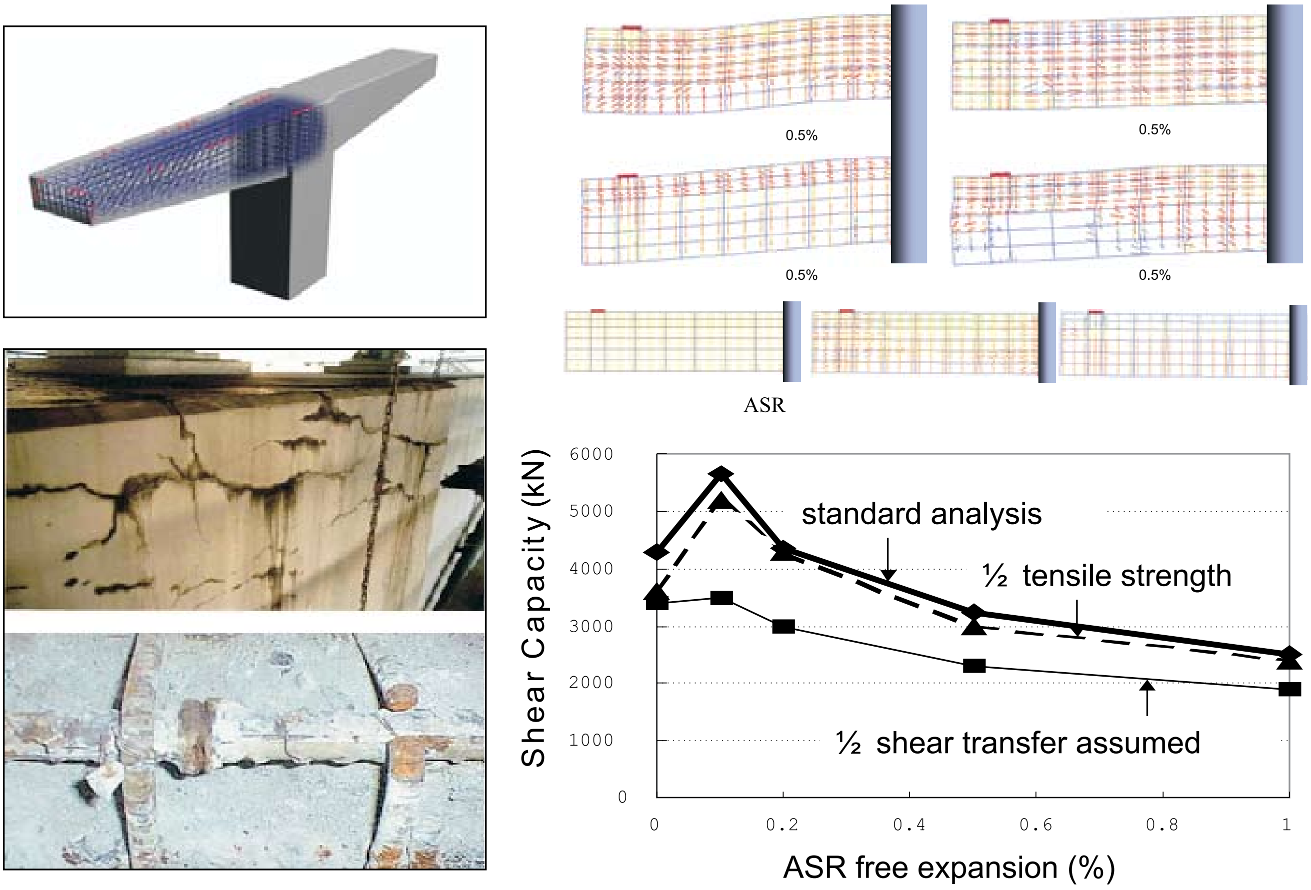
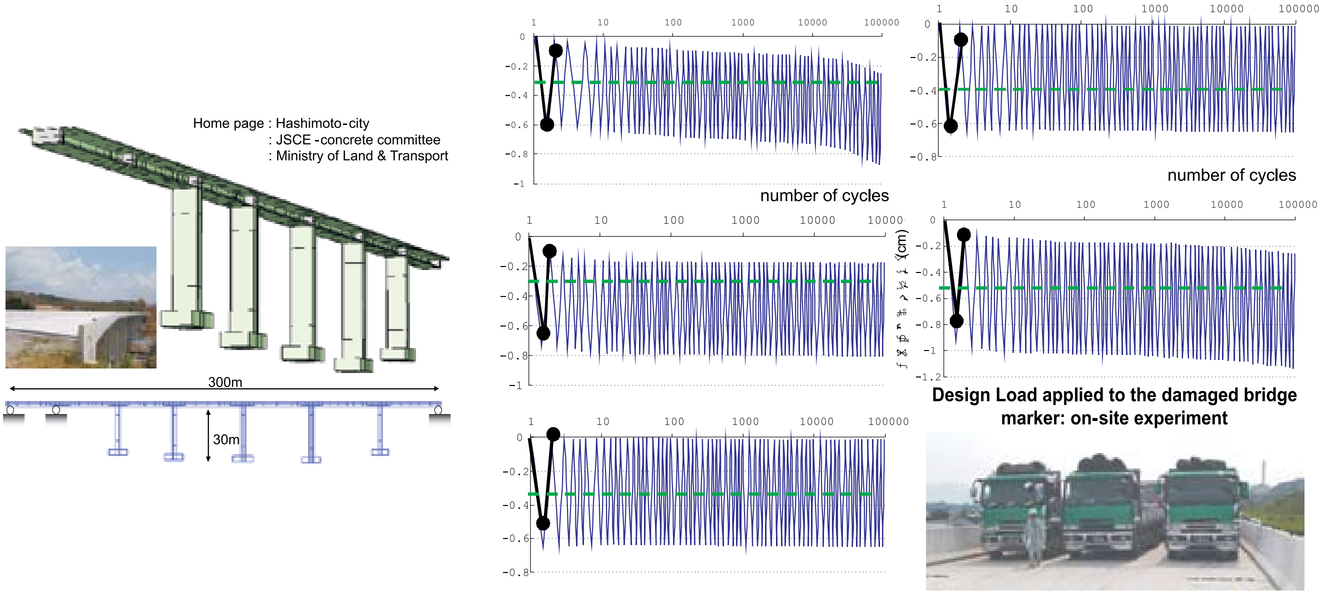
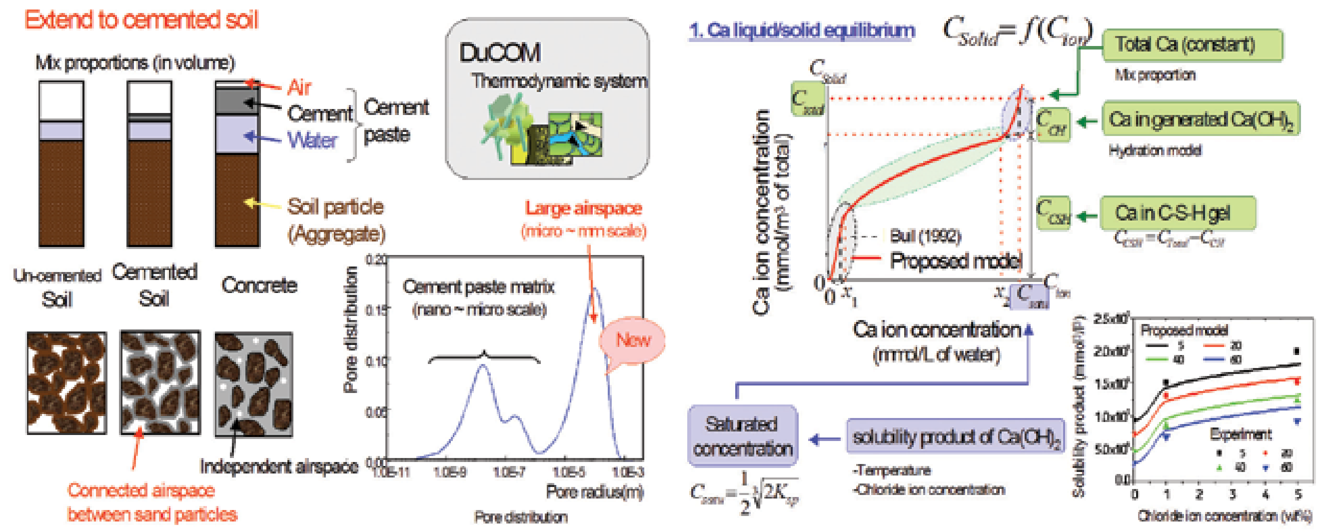


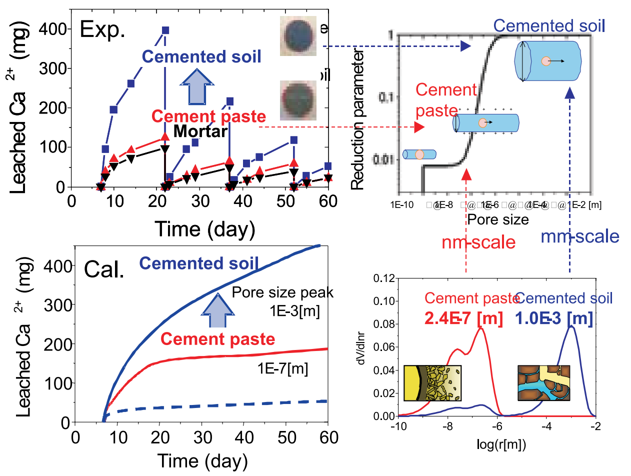
**Figure 14 – Shrinkage cracking and RC bridge pier and fatigue simulation**



### Figure 15 – Extension of micro-pore model and calcium leaching from CSH to soils



### Figure 16 – Calcium leaching of cemented soil



### Figure 17 – Verification of calcium leaching from concrete

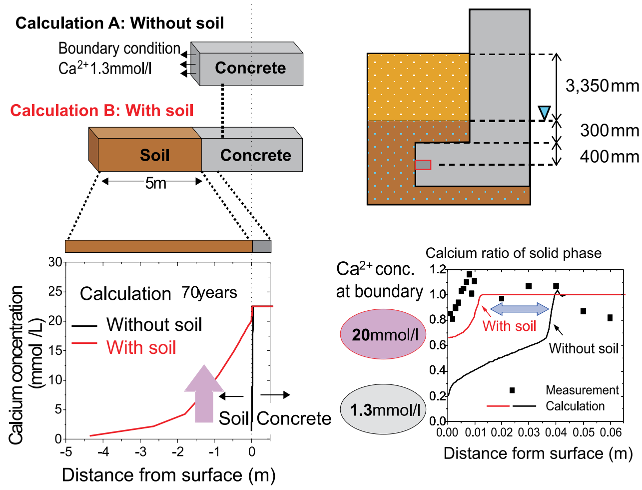


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Figure 18 – Extended calcium ion model for bentonite

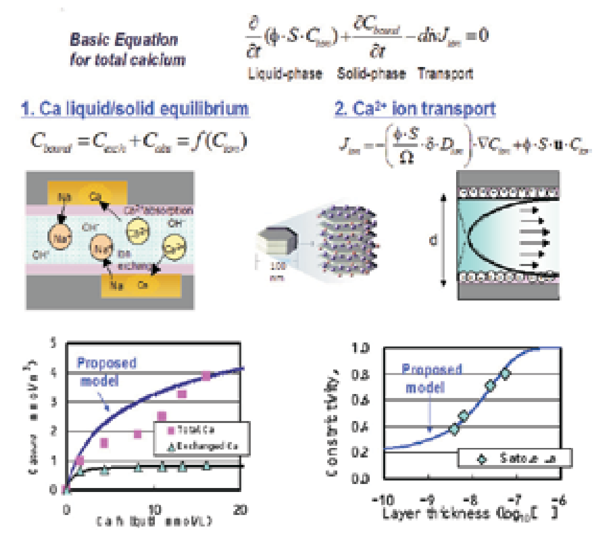
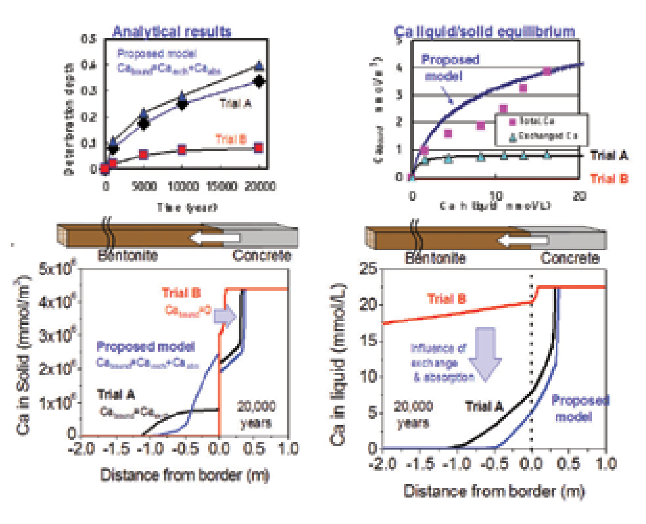


Figure 19 – Effect of bentonite on leaching of concrete



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