Multiscale lattice fracture model for cement-based materials

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Abstract

Cracking in cement-based materials is usually not easy to predict, because of the complexity of their microstructures. Concrete is a composite material of mortar and coarse aggregates, and mortar consists of cement paste and sands. The fracture processes in these materials are related, and this paper aims to reveal the relationship by developing a multiscale model using lattice approach. Lattice fracture model was proposed and applied to simulate the fracture processes in concrete in the early 1990s. Afterwards it gained extensive investigations as it can reproduce the crack patterns observed in laboratory. The lattice model can also simulate the mechanical properties of cement-based materials, such as Young's modulus, tensile strength and fracture energy. In this paper, a multiscale lattice fracture model is proposed, which can connect the fracture behavior of cement paste at microscale to the mechanical properties of mortar at mesoscale, and eventually to the performance of concrete at macroscale. The upscaling technique in this model is an implementation of the multi-level homogenization concept.

Keywords: Multiscale model, Lattice approach, Fracture in cement-based materials, Multi-level homogenization, Anm material model

Introduction

Concrete is a composite construction material, which is composed primarily of coarse aggregates, sands and cement paste. The fracture processes in concrete are complicated, because of the multiscale and multiphase nature of the material.

Among all the computational models dealing with concrete fracture, the lattice fracture model (Schlangen et al., 1997; Bolander et al., 2005; Schlangen et al., 2009; Qian et al., 2010; Qian et al., 2011) wins at several aspects, such as being able to capture detailed crack information, high computational efficiency and stability. The lattice fracture model also enables to investigate the fracture properties of concrete based on its material structure, by constructing the lattice network on top of the original material structure of concrete.

In this paper, the lattice fracture model is coupled with the parameter-passing multiscale modeling scheme to study the fracture processes in cement paste, mortar and concrete. A multiscale procedure is proposed and demonstrated. Three levels are defined, including micrometer scale for cement paste, millimeter scale for mortar and centimeter scale for concrete. The lattice fracture model is applied at each scale respectively. The inputs required at a certain scale are obtained by the simulation at a lower scale. At the lowest scale in question, the micrometer scale for cement paste, inputs for the simulation are determined by laboratory experiments and/or nanoscale modeling from literature. An example is given to show the application of the multi-level homogenization concept. The final simulated mechanical properties of concrete at centimeter scale seem to be realistic and reasonable, though not all stages of the multiscale modeling can be verified directly by laboratory experiments.

Parameter-passing scheme

Crack localization occurs during the fracture processes of cement-based materials and influences the mechanical behaviors. The phenomenon is observed in laboratory and must be reproduced in numerical experiments. One possible solution is to study the mechanical performance of cement paste, mortar and concrete at their own scale respectively, with some parameters passing from lower level to higher level. For instance, uniaxial tensile tests are simulated at micrometer scale for cement paste, millimeter scale for mortar and centimeter scale for concrete respectively, by employing the 3D lattice fracture model. These three scales are connected, and the simulated output properties of cement paste from micrometer scale modeling are used as the input properties for mortar performance evaluation at the millimeter scale, and then a similar passing takes place again from millimeter scale to centimeter scale. Hence the parameter-passing multiscale modeling scheme is established, as illustrated in Figure 1.

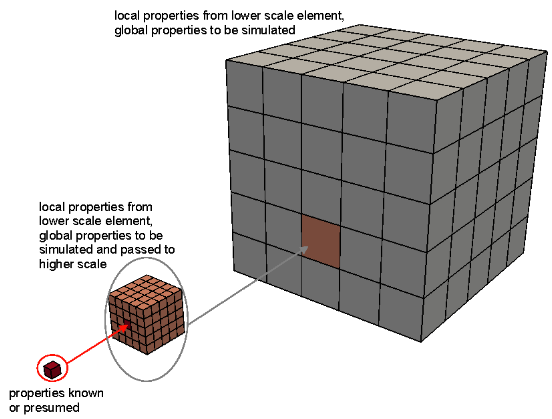


Figure 1: Parameter-passing multiscale modeling scheme

An example is given below to illustrate the application of the aforementioned scheme. A normal concrete mix is given in Table 1, and it is used to simulate the microstructure of cement paste by the HYMOSTRUC3D model (van Breugel 1997; Ye 2003) and the material mesostructures of mortar and concrete by the Anm material model (Garboczi 2002; Qian et al., 2012) respectively. The specimens at the curing age of 28 days are taken for the mechanical performance evaluation through the parameter-passing scheme. The scale division is given in Table 2. Some conditions need to be satisfied when determining the scale division. It is suggested that the specimen size should be at least 2.5 times larger than the largest particle (Garboczi et al., 1999), and the mesh size should be smaller than the smallest particle. The connecting length between cement paste and mortar is 100 μm, thus the upscaling can be done seamlessly. However, there is some length scale overlap between mortar and concrete, and domain decomposition technique is employed to solve this problem.

Table 1: A normal concrete mix

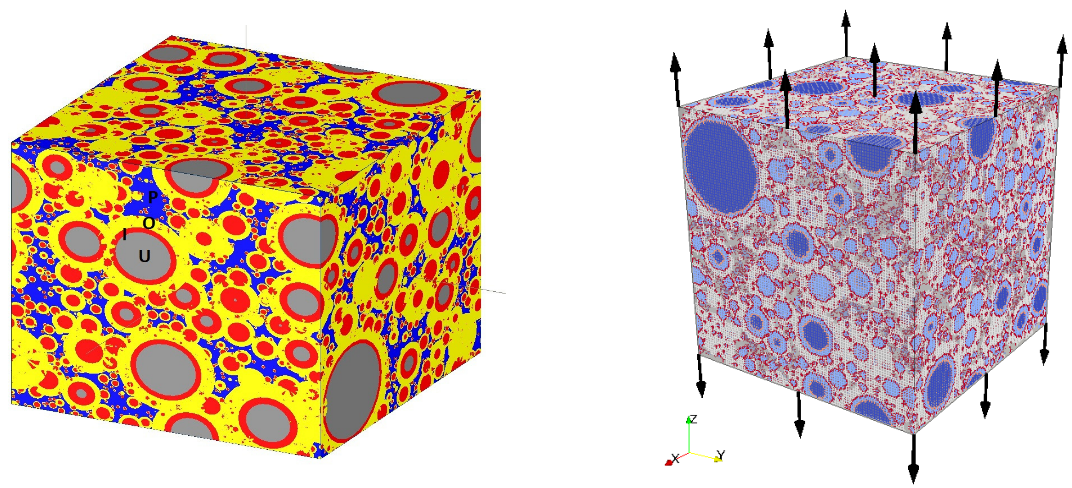
Crushed stones (≥ 4 *mm*)	786 kg/m^3	Grading:	
Uncrushed sands (< 4 *mm*)	983 kg/m^3	Crushed stones: 786 kg/m^3	
Cement	463 kg/m^3	[8, 16) *mm*	503 kg/m^3
Water	185 kg/m^3	[4, 8) *mm*	283 kg/m^3
		Uncrushed sands: 983 kg/m^3	
Concrete mass density	2417 kg/m^3	[2, 4) *mm*	270 kg/m^3
Water/cement ratio	0.4	[1, 2) *mm*	252 kg/m^3
		[0.5, 1) *mm*	192 kg/m^3
Stone and sand mass density	2650 kg/m^3	[0.25, 0.5) *mm*	153 kg/m^3
Cement mass density	3150 kg/m^3	[0.125, 0.25) *mm*	116 kg/m^3

Table 2: Scale division and specifications of the specimens

	Cement paste	Mortar	Concrete
Specimen size	$100\times100\times100$ μm	$10\times10\times10$ *mm*	$40\times40\times40$ *mm*
Mesh size	$1\times1\times1$ μm	$0.1\times0.1\times0.1$ *mm*	$1\times1\times1$ *mm*
Minimum particle size	1 μm	0.125 *mm*	4 *mm*
Maximum particle size	37 μm	4 *mm*	16 *mm*

Connecting cement paste to mortar, and then to concrete

The microstructure of a cement paste specimen of the size $100\times100\times100$ μm at the curing age of 28 days is simulated by the HYMOSTRUC3D model, as shown in Figure 2(a), and then its tensile mechanical performance is evaluated by simulating a uniaxial tensile test using lattice approach, as demonstrated in Figure 2(b). The input mechanical properties of each phase and interfaces in the microstructure are given in Table 3 [Qian 2012]. The resulting stress-strain curve is approximated by a multi-linear curve, as shown in Figure 3. The multi-linear curve will be used as the input mechanical properties of cement paste for the mortar properties prediction at the millimeter scale.



(a) Microstructure of cement paste sized at $100\times100\times100$ μm

(b) Lattice mesh at the resolution of 1 μm **and tensile test configuration**

Figure 2: Simulation of cement paste mechanical properties at micrometer scale

The points should be chosen in such a way that makes the change of input properties gradual in terms of Young's modulus and tensile strength, as listed in Table 4.

Table 3: Mechanical properties of each phase and interfaces in the cement paste at micrometer scale

No	Element type	Young's modulus E (GPa)	Shear modulus G (GPa)	Tensile strength f_t (GPa)
1	Unhydrated cement	135	52	1.8
2	Inner product	30	12	0.24
3	Outer product	22	8.9	0.15
4	Interface U-I	49	20	0.24
5	Interface I-O	25	10	0.15
6	Interface O-U	38	15	0.15

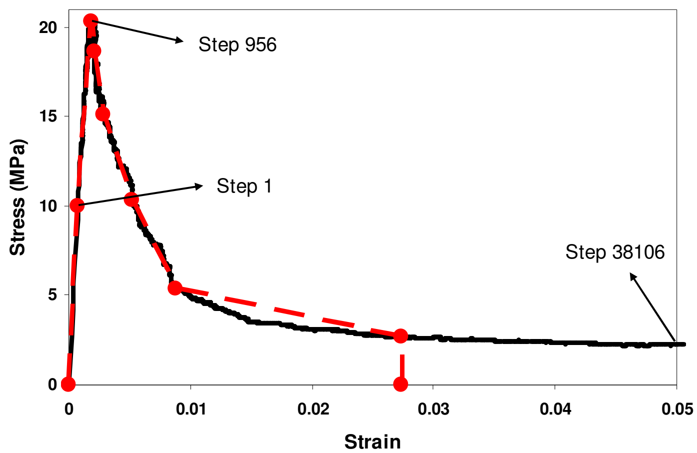
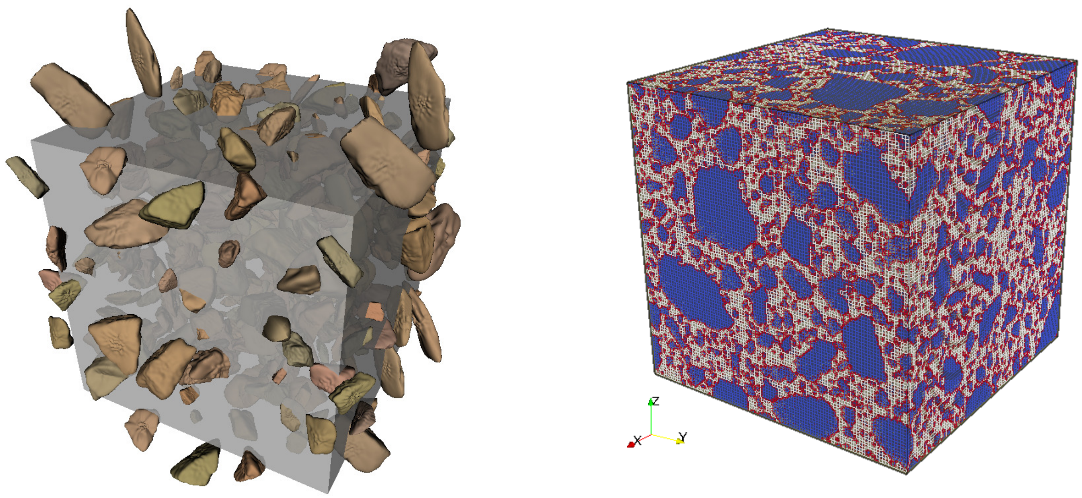


Figure 3: Simulated stress-strain curve and its multi-linear approximation for cement paste

Table 4: Mechanical properties of the cement paste specimen of the size $100 \times 100 \times 100\ \mu m$

Point	1	2	3	4	5	6	7
Young's modulus E (MPa)	12846	11096	7601	3627	1590	611	87
Shear modulus G (MPa)	5265	4548	3115	1486	652	250	36
Tensile strength f_t (MPa)	10	20	18.6	15.1	10.3	5.4	2.7

The mesostructure of mortar of the size $10 \times 10 \times 10\ mm$ is simulated by the Anm material model, as shown in Figure 4(a). The resulting mesostructure is then digitized to facilitate the subsequent lattice network construction. In the mesostructure of mortar, two solid phases are presented, namely cement paste and sand. The lattice mesh size is $0.1\ mm$, as shown in Figure 4(b), making sure that the properties of cement paste can be passed to mesoscale modeling seamlessly from microscale modeling. Three types of lattice elements are defined during the lattice network mesh, which represent sand (uncrushed US sand C109), cement paste and interface respectively. The corresponding local mechanical properties are given in Table 5 [Qian 2012].



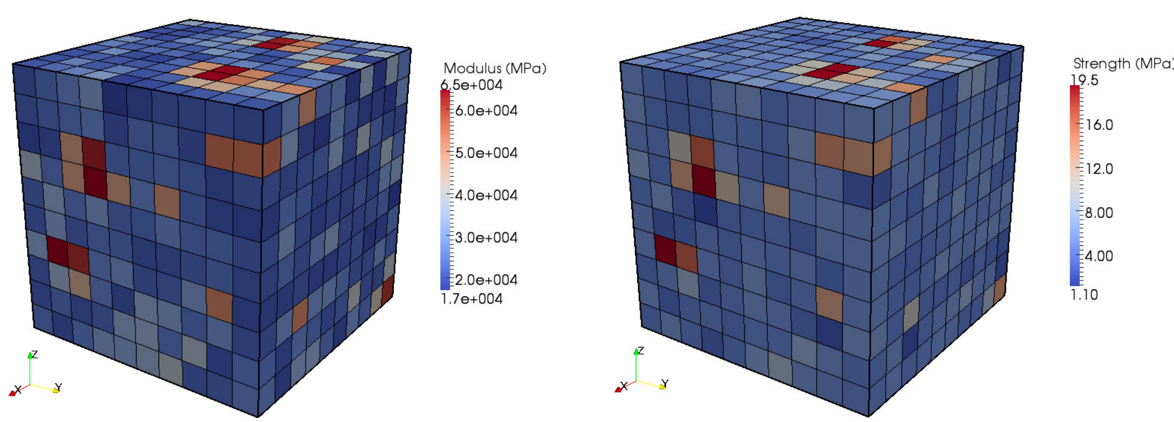
(a) Mesostructure of mortar sized at $10\times10\times10\ mm$ **(b) Lattice mesh at the resolution of** $0.1\ mm$

Figure 4 Simulation of mortar mechanical properties at millimeter scale

Table 5: Local mechanical properties of sand, cement paste and interface elements in mortar

No	Element type	Young's modulus E (GPa)	Shear modulus G (GPa)	Tensile strength f_t (MPa)
1	Sand (uncrushed)	70	29	24
2	Cement paste		multi-linear, see Table 4	
3	Interface	22	8.9	0.75

The lattice system in Figure 4(b) is decomposed to a network of blocks. The size of a single block is $1\times1\times1\ mm$, thus there are 10 blocks per direction in the original lattice system and in total 1000 blocks. Uniaxial tensile tests are simulated on these blocks one after one, using the local mechanical properties of cement paste from micrometer scale modeling. The resulting mechanical responses are scattered as the material structures of blocks may differ a lot. The simulated Young's modulus and tensile strength of every block are shown in Figure 5.



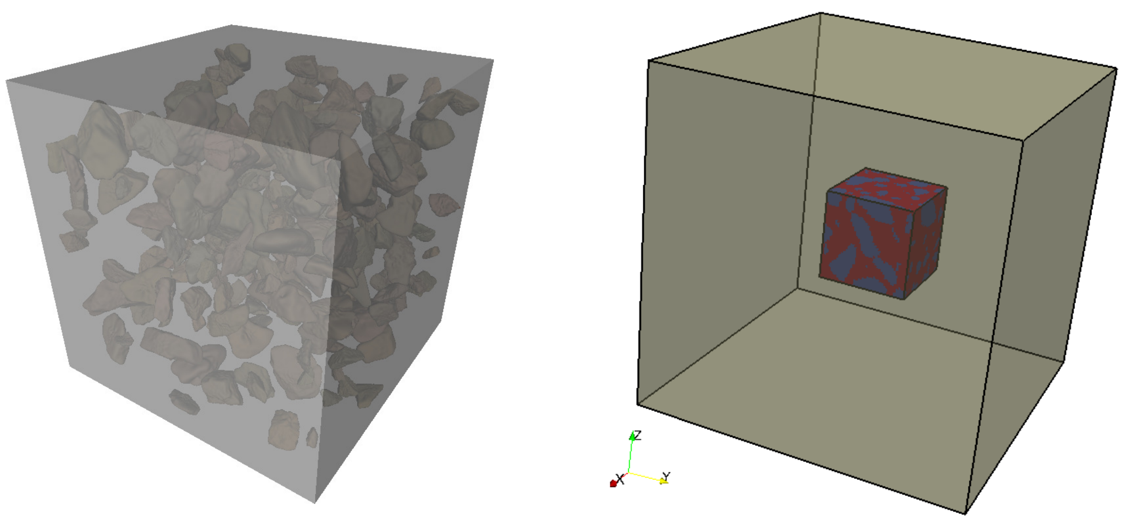
(a) Young's modulus map **(b) Tensile strength map**

Figure 5: Simulated Young's modulus and tensile strength of every block $1\times1\times1\ mm$ **in the** $10\times10\times10\ mm$ **mortar at millimeter scale**

The simulated Young's modulus of a $1\times1\times1\ mm$ block is in the range of $17\sim65\ GPa$ and averaged at $29\ GPa$. The tensile strength is in the range of $1.1\sim19.5\ MPa$ and averaged at $5.8\ MPa$. The stress-strain responses of these blocks are randomly passed onto concrete mesomechanical modeling and serve as inputs there, as elaborated below.

Having obtained the mechanical properties of the $1\times1\times1\ mm$ mortar blocks, it is ready to proceed with the concrete mesomechanical modeling. The mesostructure of concrete sized at $150\times150\times150\ mm$ is simulated by the Anm material model, as presented in Figure 6(a). A small piece of concrete of the size $40\times40\times40\ mm$ is cut out from the original simulated $150\times150\times150\ mm$ concrete specimen at its center, as shown in Figure 6(b). The $40\times40\times40\ mm$ concrete specimen is then digitized at the resolution of $1\ mm$, and consists of two solid phases namely stone and mortar. A lattice network is constructed based on the digital concrete specimen, and three types of lattice elements are identified, which represent crushed stone, mortar and interface respectively, as shown in Figure 7(a). The local mechanical properties are given in Table 6 [Qian 2012]. The properties of mortar come from millimeter scale modeling and are varied according to the simulation results of $1\times1\times1\ mm$ mortar blocks.

A uniaxial tensile test is simulated on the lattice system meshed from the $40\times40\times40\ mm$ concrete specimen, as shown in Figure 7(a). The resulting stress-strain response is presented in Figure 7(b), and some mechanical properties can be computed as given in Table 7.



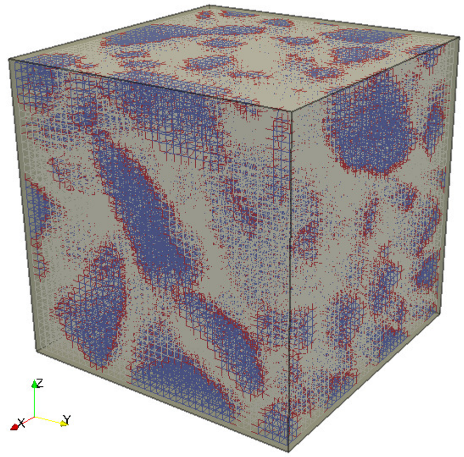
(a) Original specimen sized at $150\times150\times150mm$

(b) A cut-out specimen sized at $40\times40\times40mm$

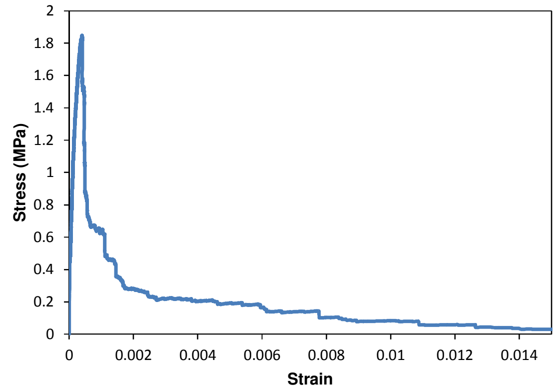
Figure 6: Mesostructures of concrete at centimeter scale

Table 6: Local mechanical properties of stone, mortar and interface elements in concrete

No	Element type	Young's modulus E (GPa)	Shear modulus G (GPa)	Tensile strength f_t (MPa)
1	Stone (crushed)	70	29	24
2	Mortar	multi-linear and varied based on the $1\times1\times1\ mm$ mortar blocks		
3	Interface	41	17	1



(a) Lattice mesh of the cut-out specimen $40 \times 40 \times 40\ mm$ **at the resolution of** $1\ mm$



(b) Simulated stress-strain curve

Figure 7 Simulation of concrete mechanical properties at centimeter scale

Table 7 Simulated mechanical properties of concrete at centimeter scale

Young's modulus E (GPa)	Tensile strength f_t (MPa)	Strain at peak load ε_p	Fracture energy G_F (J/m^2)
31	1.8	0.04%	127

The pattern of the simulated stress-strain response of $40 \times 40 \times 40\ mm$ concrete is similar to the one observed in laboratory, and the mechanical properties computed from the stress-strain diagram are also located within the reasonable range.

Conclusions

In this paper, the parameter-passing multiscale modeling scheme is combined with the lattice fracture model to evaluate the mechanical performance of concrete using a multiscale approach. The integrated system of cement paste, mortar and concrete is separated and analyzed at different scales. The material structures of cement paste, mortar and concrete are simulated by the HYMOSTRUC3D model and the Anm material model respectively. The 3D lattice fracture model is used to evaluate their mechanical performance by simulating a uniaxial tensile test. The simulated output properties at a lower scale are passed onto a higher scale to serve as local input properties. Domain decomposition technique is employed to solve the length scale overlap between mortar and concrete. Thus a three-level multiscale lattice fracture analysis is performed. The final simulation results at mesoscale seem to be reasonable and realistic, and must be further verified by experiments in laboratory in future. The combination of the 3D lattice fracture model and the parameter-passing scheme, thus the multiscale lattice fracture model, enables the study on cement-based materials through a multiscale approach, which is proved to be a successful initiative in this paper.

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References

Bolander, J.E. and Sukumar, N. (2005), Irregular lattice model for quasistatic crack propagation. Phys. Rev. B. 71, 094106.

Garboczi, E.J. (2002), Three-dimensional mathematical analysis of particle shape using X-ray tomography and spherical harmonics: Application to aggregates used in concrete. Cement and Concrete Research. 32, pp. 1621–1638.

Garboczi, E.J. and Bentz, D.P. (1999), Computer Simulation and Percolation Theory Applied to Concrete. Annual Reviews of Computational Physics VII. World Scientific Publishing Company. pp. 85–123.

Qian, Z. (2012), Multiscale Modeling of Fracture Processes in Cementitious Materials. PhD thesis. Delft University of Technology.

Qian, Z., Schlangen, E., Ye, G. and van Breugel, K. (2010), Prediction of Mechanical Properties of Cement Paste at Microscale. Materiales de Construccion. 60, pp. 7–18.

Qian, Z., Schlangen, E., Ye, G. and van Breugel, K. (2011), 3D Lattice Fracture Model: Theory and Computer Implementation. Key Engineering Materials. 452-453, pp. 69–72.

Schlangen, E. and Garboczi, E.J. (1997), Fracture simulations of concrete using lattice models: Computational aspects. Engineering Fracture Mechanics. 57, pp. 319–332.

Schlangen, E. and Qian, Z. (2009), 3D modeling of fracture in cement-based materials. Journal of Multiscale Modelling. 1, pp. 245–261.

van Breugel, K. (1997), Simulation of Hydration and Formation of Structure in Hardening Cement-based Materials. PhD thesis. Delft University of Technology.

Ye, G. (2003), Experimental Study and Numerical Simulation of the Development of the Microstructure and Permeability of Cementitious Materials. PhD thesis. Delft University of Technology.