4 Sensitivity Analysis for Some Composites

4.1 Deterministic Problems

As is known, the sensitivity analysis in engineering systems is employed to verify how input parameters of a specific engineering problem influence the analysed state functions (displacements, stresses and temperatures, for instance). The sensitivity coefficients [269], being the purpose of such an analysis, are computed using partial derivatives of the considered state function with respect to the particular input parameter(s). These derivatives can be obtained numerically starting from the fundamental algebraic equations system of the problem, for instance, or alternatively, by a simple derivation if only a closed form solution exists; some combined analytical−numerical methods are also known [99]. It is important to underline that this methodology is common for all discrete numerical techniques: Boundary Element Method (BEM) [51,206], Finite Difference Method (FDM) [90,206], FEM [7,21,387] as well as hybrid and meshless strategies [81].

From the computational point of view, there are the following numerical methods in structural design sensitivity analysis [75,76,103,134,207]: the Direct Differentiation Method (DDM), the Adjoint Variable Method (AVM) applied together with the Material Derivative Approach (MDA) or the Domain Parametrisation Approach (DPA) suitable for shape sensitivity studies. Considering these capabilities and, on the other hand, a very complex structure of composite materials, sensitivity analysis should be applied especially in design studies for such structures. Instead of a single (or two) parameters characterising the elastic response of a homogeneous structure, the total number of design parameters is obtained as a product of component numbers in a composite and the number of material and geometrical parameters for a single component. Even some extra state variables should be analysed to define interfacial behaviour, general interaction of the constituents and/or the lack of periodicity. Usually, to reduce the complexity of the original composite, the so−called effective homogenisation medium having the same strain (or complementary) energy is analysed.

This chapter is devoted to general computational sensitivity studies of the homogenisation method for some periodic composite materials with linear elastic and transversely isotropic constituents. The composite is first homogenised, the effective material tensor components are computed using the FEM−based additional computer program. Further, material parameters of the composite most decisive for its effective material properties are determined numerically. It should be underlined that the homogenisation method is generally an intermediate numerical tool applied to exclude the necessity of composite micro−scale discretisation and, in the same time, to reduce the total number of degrees of freedom of the entire model. On the other hand, there are many numerical homogenisation techniques. They can be divided generally into two essentially different approaches: stress averaging (the boundary stresses are introduced between the composite constituents plus displacement−type periodicity conditions) and strain approach (uniform extensions of the RVE boundaries in various directions plus periodicity conditions on the remaining cell edges). Considering this, different results of the homogenisation method in terms of the effective material tensors are obtained (as a result quite different sensitivity gradients must be computed in these two approaches). The sensitivity analysis introduces a new aspect of the homogenisation technique – it can be verified if the homogenised and original structures have the same or even analogous (in terms of their signs) sensitivity gradients. The composites can be optimised then by manipulating its material or geometrical design parameters [310] as well as by choosing various constituent materials with computationally determined shape for the new designed composite structure.

The sensitivity gradients are computed here by application of a homogenisation−oriented computer program MCCEFF according to the DDM implementation approach and presented as functions of the composite design parameters − Young moduli and Poisson ratios of the constituents. Since a finite difference scheme is used for the sensitivity gradient computations, numerical sensitivity of the final results to the increase of an arbitrarily introduced parameter must be verified. This numerical phenomenon makes it necessary to determine the most suitable interval of parameter increments for the particular effective elasticity tensor components.

The entire computational methodology is illustrated with two examples – 1D and 2D two component periodic composites. The closed form effective Young modulus is used in the first example, while the homogenisation function is to be computed in the second case. Both illustrations show that different components of the effective elasticity tensor show different sensitivities to particular mechanical properties of the original composite and, further, the illustrations make it possible to determine the most decisive elastic parameters for the homogenisation−based computational design studies. Quite similar sensitivity studies are carried out in the case of heat conductivity coefficient for 1D, 2D and 3D two component composites.

It should be noticed that sensitivity analysis can be used for validation of various homogenisation methods. In most cases an increase in Young moduli of composite components should result in a corresponding increase of the effective material tensor components; an opposite phenomenon can be observed for some specific cases, but usually in an extremely small range only. Therefore, if the sensitivity analysis shows that most of the gradients are negative, the homogenisation theory should be essentially corrected.

The applied effective modulus method is verified below using the examples of 1D distributed heterogeneities in the periodic two−component bar structure and of the fibre−reinforced periodic composite. As is demonstrated for plane composite structure, the sensitivity gradients of a homogenised elasticity tensor show some instabilities observed for an extremely small value of the perturbation parameter.

At the same time, for Poisson ratios values tending to their physical bounds, an uncontrolled increase of all sensitivity gradients is observed. That is why a continuation of this study is necessary in the context of computational error, to extend constitutive models of composite components as well as to evaluate geometrical and material sensitivity gradients for more complex heterogeneous structures, especially in the probabilistic context.

Another important topic studied here is the application of the parameter finite difference analysis to the sensitivity analysis of the uniform plane strain problem of the real composite. This is done under the assumption that the RVE of plane cross–section is uniformly extended in two perpendicular directions and the unit shear strain is applied on the RVE. Therefore, the sensitivity functional is proposed as the elastic strain energy stored in the cell, which is treated as some type of representative strain state of the composite under real conditions. To reflect the real conditions of the composite service more accurately, the particular strain component can be scaled over some multipliers to illustrate pure horizontal and/or vertical extension of the composite specimen. The sensitivity of this functional is taken as a measure of influence of various material parameters on the overall behaviour of the composite. According to the previous results, we observe the Poisson ratio of the matrix as a dominating material parameter for the fibre–reinforced periodic composites with the RVE specified below.

Finally, it should be mentioned that this sensitivity analysis is introduced and performed to validate the homogenisation theory itself. In the case when the external boundary conditions are known together with the micromorphology of a certain composite, the homogenisation theory makes it possible to determine the effective characteristics of this structure and, according to the sensitivity analysis the sensitivity gradients of both real and homogenised structures are computed. If these gradients have consistent signs and comparable values, the homogenisation algorithm proposed is useful in computational modelling; otherwise another method should be proposed. It can happen that some homogenisation theories (or even closed form equations) are valid for some specific boundary value problems and it can be verified in this way. Another promising field of application of such an analysis is optimization and/or identification of composite materials and structures.

Sensitivity gradients cannot be obtained analytically if the homogenisation function components are determined numerically in some cell problem solutions. Hence, two separate ways can be followed, the first one being purely computational finite difference based studies, where the gradients are obtained as differences of some slightly modified homogenisation tests. Alternatively, a semi–analytical method can be implemented where the spatial averages of the constitutive tensor components (independent from homogenisation functions) are differentiated symbolically and the remaining part resulting from homogenisation FEM tests is analysed using the finite differences; analogous opportunities are available for probabilistic (and next stochastic) analyses. Taking into account the consistency of the Monte Carlo simulation application and the computational time savings, full numerical differentiation is implemented. A semi–analytical approach can be implemented partially in some mathematical symbolic computation packages, where probabilistic moments can be derived according to the classical integral definitions, while the random fields of homogenising stresses averaged over the RVE are treated using the numerical differentiation approach.

The results of computations in the form of deterministic derivatives or their probabilistic equivalents can next be implemented in deterministic and/or probabilistic optimisation problems based on the gradient techniques. Such an analysis will enable us to optimise various composites [84,240,264,281,320] using their homogenised models – without the necessity of complicated multiscale problem discretisation and their further solution. The main benefits of the integrated computational approach to the composites are (a) the most effective choice of composite components (sensitivity to the expected values of material parameters), (b) selection of the best processing technology from the necessary accuracy point of view (standard deviation levels), (c) efficient durability control and analysis (sensitivity to the interface and structural defects parameters), etc. The proposed method is significantly more complicated than the previous approaches. However it makes the computational model of composite materials and their behaviour more realistic and focused on the engineering analyses.

4.1.1 Sensitivity Analysis Methods

The main aim of the structural design sensitivity analysis is to study the interrelation between the response (or state variables) of a structure determined from a solution for the boundary–value problem and design variables begin the input data for the solution process. Displacements, stresses, temperatures or velocities can be taken as the structural response measures, whereas such parameters as truss and beam cross–sectional areas, plate and shell thicknesses and material characteristics are usually chosen as design variables. Let us note that even for linear elastic problems the equilibrium equations may generally contain some nonlinear expressions for the state and design variables – this is the case of plate/shell thickness and/or truss lengths and, especially, material parameters in composites.

The sensitivity gradients are the main numerical tool to evaluate the design sensitivity of a structure with respect to some design parameter. For engineers a more interesting issue is the overall sensitivity of the structure examined under general loading conditions than particular state function gradients. The gradients of the structural response functionals with respect to design variables give a useful measure of structural response variation together with the change of a given design input.

The sensitivity analysis is especially applicable with common implementation with one of the well-established numerical methods of structural analysis, i.e. with the finite element formulation. To illustrate the main ideas let us consider the static structural response of a linear elastic system with N degrees of freedom defined by the functional [208]

$$\Im\left(h^d\right)=G\left[q_\alpha\left(h^d\right),h^d\right],\quad d=1,2,\ldots,D;\quad \alpha=1,2,\ldots,N \tag{4.1}$$

where G is a given function of structural displacements vector (q_α) and design variables, h^d represents a D−dimensional vector of design variables; the displacement vector satisfies classical equilibrium equations, i.e.

$$K_{\alpha\beta}\left(h^d\right)q_\beta\left(h^d\right)=Q_\alpha\left(h^d\right) \tag{4.2}$$

The displacement vector is assumed to be an implicit function of design variables, because the stiffness matrix $K_{\alpha\beta}$ and the load vector Q_α are some functions of these variables.

Now, the SDS analysis is employed to determine the changes of the structural response functional with variations in design parameters, so the so−called sensitivity gradient $\partial\Im/\partial h^d$ is to be determined. The chain rule of differentiation applied to (4.1) returns here

$$\Im^{,d}=G^{,d}+G_{,\alpha}q_\alpha^{,d} \tag{4.3}$$

where $(.)^{,d}$ and $(.)_{,\alpha}$ denote first partial derivatives with respect to the dth design variable and the αth nodal displacement, respectively. The design variables h^d are introduced as the only arguments in the functions $\Im$, $K_{\alpha\beta}$, q_α , Q_α and, therefore, partial derivatives of these functions with respect to h^d are in fact equal to the corresponding total derivatives. Nevertheless, there holds $\partial G/\partial h^d=\Im^{,d}$ in case of G. Since it is an explicitly given function of h^d and q_α , the derivatives $G^{,d}$ and $G_{,\alpha}$ may be computed directly, while $q_\alpha^{,d}$ is to be determined numerically.

The first technique for computing of the sensitivity gradients known as the direct differentiation method (DDM) extensively employed in structural optimisation reflects the following algorithm. Let us assume that $K_{\alpha\beta}\left(h^d\right)$ and $Q_\alpha\left(h^d\right)$ are continuously differentiable with respect to the design variables h^d ; then, the vector $q_\beta\left(h^d\right)$ is also continuously differentiable. Differentiation of both sides of (4.2) with respect to h^d gives

$$K_{\alpha\beta}q_\beta^{,d}=Q_\alpha^{,d}-K_{\alpha\beta}^{,d}q_\beta \tag{4.4}$$

Since the stiffness matrix $K_{\alpha\beta}$ is assumed to be nonsingular, (4.4) can be solved for $q_\beta^{,d}$; it yields

$$\Im^{.d} = G^{.d} + G_{.\beta} K_{\alpha\beta}^{-1} \left(Q_{\alpha}^{.d} - K_{\alpha\gamma}^{.d} q_{\gamma} \right) \tag{4.5}$$

The alternative AVM strategy begins with the introduction of an adjoint variable vector λ_α, α=1,2,…,N such that

$$\lambda_\alpha = G_{.\beta} K_{\alpha\beta}^{-1} \tag{4.6}$$

It yields the adjoint equations for λ_α in the form

$$K_{\alpha\beta} \lambda_\beta = G_{.\alpha} \tag{4.7}$$

and then, the sensitivity gradient coefficients may be obtained as

$$\Im^{.d} = G^{.d} + \lambda_\alpha \left(Q_{\alpha}^{.d} - K_{\alpha\beta}^{.d} q_{\beta} \right) \tag{4.8}$$

having solved the above equation for the adjoint variables λ_β. The main ideas of the DDM and AVM seem to be identical but in realistic engineering design problems their computer performance is considerably different. Since most of the functions are given explicitly in the problems considered, the DDM technique has found its application below.

The matrices of derivatives of practically any order of the global stiffness matrix with respect to design variables are obtained simply by adding derivatives of element stiffness expressed in the global coordinate system. It is done quite similarly to the assembling procedure for the global stiffness matrix. This process is usually essentially simplified, because almost all entries in the matrices of their derivatives with respect to the particular design variables are equal to 0 and then all arithmetic operations can be carried out at the element level.

Effective computation of stiffness derivatives with respect to design variables for finite elements is another issue to be taken into account in developments of any sensitivity-oriented software. Most up-to-date finite element codes engage numerical integration instead of using the closed form expressions in terms of design variables to generate the element stiffness matrices. For such numerically generated element matrices a differentiation process with respect to design variables can be performed through a sequence of computations (at least two solution for initial and for a slightly perturbed design parameter) used to generate these matrices, leading to implicit design derivative procedures.

The element matrices of the design derivatives can also be obtained by using a finite difference scheme, which is demonstrated for the eth element of the stiffness matrix

$$\frac{\partial K_{\alpha\beta}^{(e)}}{\partial h^{\bar{d}}} \cong \frac{1}{\varepsilon} \left[K_{\alpha\beta}^{(e)} \left(h + 1_{(\bar{d})} \varepsilon \right) - K_{\alpha\beta}^{(e)} (h) \right], \; \bar{d} = 1,2,\ldots,D, \tag{4.9}$$

where $K_{\alpha\beta}^{(e)}$ is the eth element stiffness matrix, $h^{\bar{d}}$ is the $\bar{d}$ th component of the D−dimensional design variable vector h, ε represents a small perturbation and the D−dimensional vector $1_{(\bar{d})}$ is equal to 1 at the $\bar{d}$ th position and zeroes elsewhere. Such a scheme is known as forward finite difference rule, however backward and central differences can be applied too. Backward differentiation uses the values of a function in actual (h) and previous point (h-ε), while central difference is returned from arithmetic averaging of equations containing forward and backward differences.

4.1.2 Sensitivity of Homogenised Heat Conductivity

As is known, it is possible to obtain the effective heat conductivity tensor components by the application of some algebraic approximations for particular types of composite materials. However, numerical procedure is not very general in this case. The effective heat conductivity for a periodic fibre−reinforced composite in a 2D problem where the fibre has the round cross−section and the total composite volume is relatively large in comparison to the single inclusion can be approximated using the Cylinder Assemblage Model (CAM) for a fibre−reinforced plane structure. The Spherical Inclusion Model (SIM) [65] for spherical inclusions distributed periodically (3D composite). The heat conductivity coefficients of composite components k_1, k_2 are such that $k_1>k_2$ (the same results hold true for electrical conductivity, magnetic permeability and the dielectric constant for composites, for instance).

A concept of the first test is to compare the effective heat conductivities obtained for the 1D, 2D (fibre) and 3D (particle-reinforced) composites in terms of various reinforcement volume ratios and the interrelation between heat conductivity coefficients for both components. The following equations are used:

- 1D composite

$$k^{(eff)} = \frac{|\Omega|}{\int_\Omega \frac{d\Omega}{k(y)}}$$

- 2D composite

$$k_{2D}^{(eff)} = k_2\left(1+v_f\left(\frac{1-v_f}{2}+\frac{k_2}{k_1-k_2}\right)^{-1}\right)$$

- 3D composite

$$k_{3D}^{(eff)} = k_2\left(1+v_f\left(\frac{1-v_f}{3}+\frac{k_2}{k_1-k_2}\right)^{-1}\right)$$

where v_f is the reinforcement volume fraction, while k_1, k_2 are heat conductivity coefficients of composite components such that $k_1>k_2$.

Furthermore, the sensitivities of effective heat conductivity with respect to those characterising original composite components are determined: the computations are performed using the mathematical package MAPLE. All the results of the numerical experiments are presented in Figures 4.1–4.9: the effective heat conductivities for the 1D, 2D and 3D composites are plotted in Figures 4.1–4.3, their material sensitivities with respect to design variable k_1 in Figures 4.4–4.6, while sensitivity studies with respect to the parameter k_2 are presented in Figures 4.7–4.9.

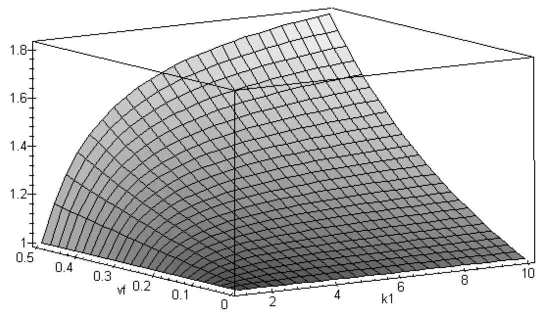

Figure 4.1. Effective heat conductivity for 1D composite

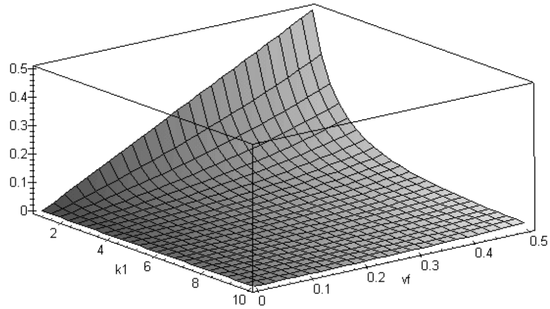

Figure 4.2. Material sensitivity of $k^{(eff)}$ in 1D problem to k_1

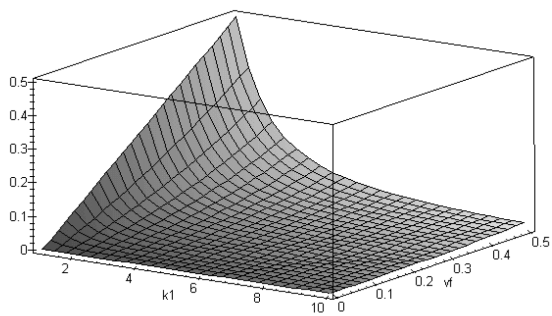

Figure 4.3. Sensitivity of $k^{(eff)}$ in 1D problem to v_f

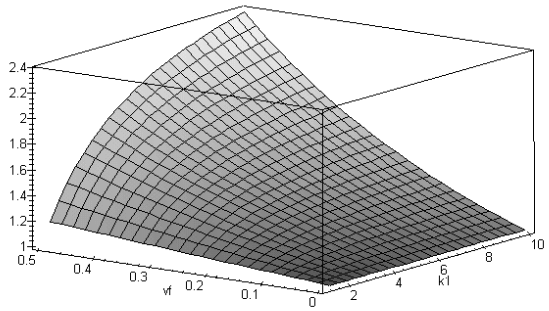

Figure 4.4. Effective heat conductivity for 2D composite

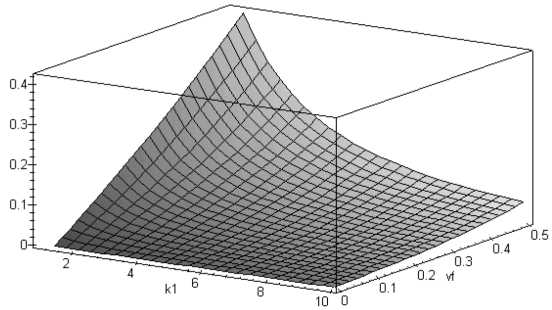

Figure 4.5. Material sensitivity of $k^{(eff)}$ in 2D problem to k_1

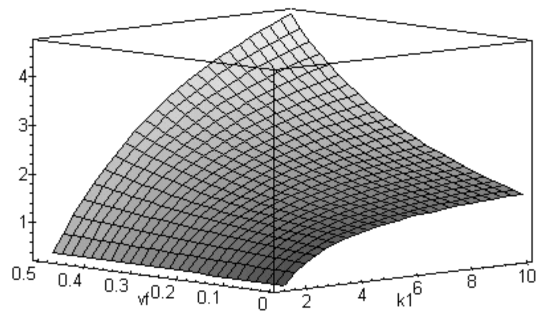

Figure 4.6. Sensitivity of $k^{(eff)}$ in 2D problem to v_f

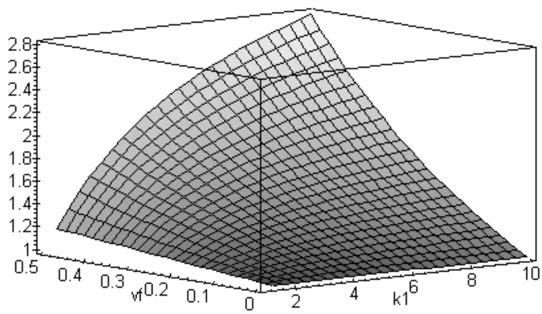

Figure 4.7. Effective heat conductivity for 3D composite

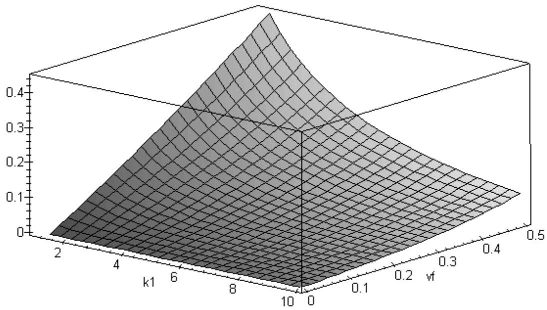

Figure 4.8. Material sensitivity of $k^{(eff)}$ in 3D problem to k_1

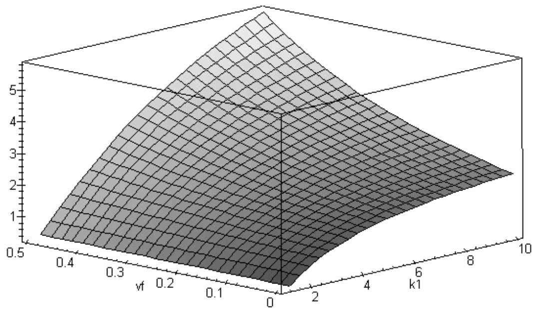

Figure 4.9. Sensitivity of $k^{(eff)}$ in 3D problem to v_f

Analysing numerical results it can be observed that the effective heat conductivity surface has an analogous shapes for 1D, 2D and 3D composites. However the values of this coefficient obtained for the same reinforcement ratio are largest for 3D composite with spherical inclusion, next largest for 2D fibre−reinforced composite, and smallest for the 1D case. Therefore, 3D composites seem to be most optimal − using the same volume of reinforcement, the highest value of the effective material property is obtained. According to engineering intuition, it is found that increasing both k_1 and v_f an increasing of final value of $k^{(eff)}$ is obtained. The results of sensitivity studies presented in Figures 4.3, 4.6 and 4.9 make it possible to observe the greatest sensitivity of composite effective characteristics with respect to both design parameters (k_1 and v_f) for extremely small values of the coefficient k_1 and the largest value of the reinforcement ratio. The sensitivity gradients of $k^{(eff)}$ with respect to v_f have almost constant value, while with respect to k_1 are efficiently nonlinear and reach the maximum forv_f=0.5 (cf. Figure 4.2 and 4.3, for instance). This result means that the effective conductivity value is most sensitive to the changes of k_1, if the reinforcement volume ratio is maximal, which is predictable result and it positively validates this homogenisation method.

The smallest sensitivity of $k^{(eff)}$ to the parameter k_1 can be noted for v_f tending to 0, while the inverse relation is observed with respect to the reinforcement volume fraction. The variability of the sensitivity surface for $k^{(eff)}$ with respect to the heat conductivity coefficient k_1 is almost the same for all composites. However in the case of sensitivity to v_f the 2D and 3D models are similar, while the 1D case is essentially different − it results from the relevant equations forms.

4.1.3 Sensitivity of Homogenised Young Modulus for Periodic Composite Bars

Let us consider periodic composite bar applied to the compressive/tensile stresses and the homogenised Young modulus of such a structure. For such a unidirectional n−component composite structure, one can readily obtain the sensitivity gradients of the effective parameter $e^{(eff)}$ with respect to the modulus of its jth component e_j as

$$\frac{\partial e^{(eff)}}{\partial e_j} = \frac{\prod_{i=1}^{j-1} e_i \prod_{j+1}^{n} e_i \left(\sum_{i=1}^{n} A_i l_i e_1 e_2 \ldots e_{i-1} e_{i+1} \ldots e_n \right)}{\left(\sum_{i=1}^{n} A_i l_i e_1 e_2 \ldots e_{i-1} e_{i+1} \ldots e_n \right)^2} - \frac{\prod_{i=1}^{n} e_i \frac{1}{e_j} \left(\sum_{i=1}^{j-1} A_i l_i e_1 e_2 \ldots e_{i-1} e_{i+1} \ldots e_n + \sum_{j+1}^{n} A_i l_i e_1 e_2 \ldots e_{i-1} e_{i+1} \ldots e_n \right)}{\left(\sum_{i=1}^{n} A_i l_i e_1 e_2 \ldots e_{i-1} e_{i+1} \ldots e_n \right)^2} \tag{4.10}$$

The geometrical sensitivity with respect to the cross-sectional area A_j is determined as

$$\frac{\partial e^{(eff)}}{\partial A_j} = -\frac{\prod_{i=1}^{n} e_i \left(l_j e_1 e_2 \ldots e_{j-1} e_{j+1} \ldots e_n \right)}{\left(\sum_{i=1}^{n} A_i l_i e_1 e_2 \ldots e_{i-1} e_{i+1} \ldots e_n \right)^2} \tag{4.11}$$

Analogously, geometrical sensitivity with respect to the member length l_j is calculated from the following formula:

$$\frac{\partial e^{(eff)}}{\partial l_j} = -\frac{\prod_{i=1}^{n} e_i \left(A_j e_1 e_2 \ldots e_{j-1} e_{j+1} \ldots e_n \right)}{\left(\sum_{i=1}^{n} A_i l_i e_1 e_2 \ldots e_{i-1} e_{i+1} \ldots e_n \right)^2} \tag{4.12}$$

It should be underlined that the equations obtained above can be relatively easily inserted in the 1D implementations of the FEM formulation for elastostatics as well as heat conduction problems, both in deterministic and stochastic computation.

Now, the sensitivity gradients are derived first for a 1D two–component composite with the RVE presented in Figure 2.42. Considering the fact that composite materials are characterised by numerous parameters, it is essential to reduce this number by introduction of non–dimensional normalised parameters between the corresponding material and geometric characteristics of a composite. It is recommended to make the sensitivity analysis more focused with opportunity to compare the sensitivity gradients with each other.

Determination of the first sensitivity gradient, cf. (4.11), makes it possible to verify how the interrelation between cross–sectional area α of both components influences the final effective Young modulus of the composite. The next gradient is responsible for the sensitivity of the composite to the length of both components ratio γ, while the last one gives information about the influence of interrelation β of the Young moduli for composite components.

The general observation in this analysis is that an increase in analysed structural geometrical parameters results in a decrease of the effective parameter value (negative derivative sign) and vice versa. Analogously, it is observed that increasing any Young modulus of composite components, the increase of the effective homogenised parameter is obtained. Quantitative verification of the most decisive parameter depends on the interrelations between particular material and geometrical characteristics and should be analysed in detail in further studies. In case of the unidirectional composite, the shape sensitivity studies with respect to the interface location can be done analytically. All the sensitivities calculated above enable us to design, during engineering studies, the most suitable interrelations between particular components for unidirectional tensioned/compressed structural members. Considering the nature of the presented 1D homogenisation approach, it is clear that the sensitivity of the Young modulus holds true for the effective heat conductivity and other related coefficients.

The first and second order sensitivity gradients together with the mean value of the homogenised Young modulus have been computed and collected in the figures below. The following input data are adopted: e_2=2.0E9, the coefficient γ relating the lengths of composite components is arbitrarily taken as equal to 1. Other parameters are adopted in the following form: A_2=0.2 and l_2=10.0. The effective Young modulus is determined with respect to the reinforcement ratio as well as to the cross-sectional area ratio of the components and presented below.

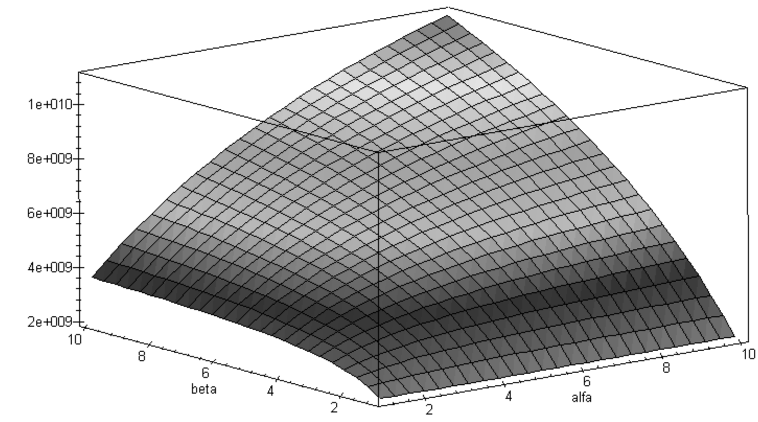

Figure 4.10. Parameter variability of the effective Young modulus

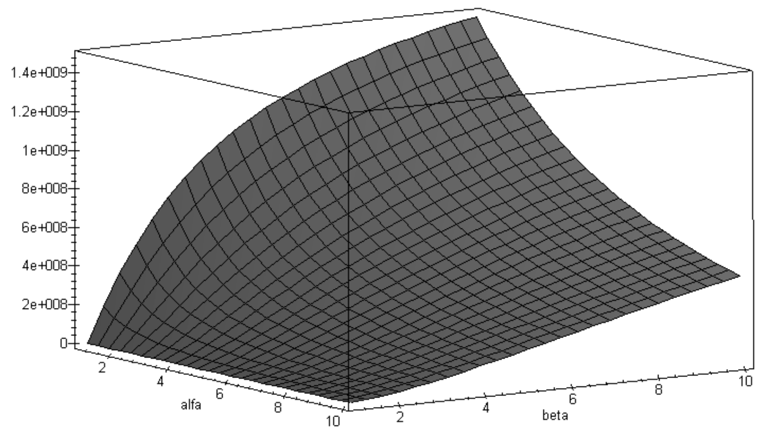

Figure 4.11. Parameter variability of $e^{(eff)}$ sensitivity gradient wrt parameter α

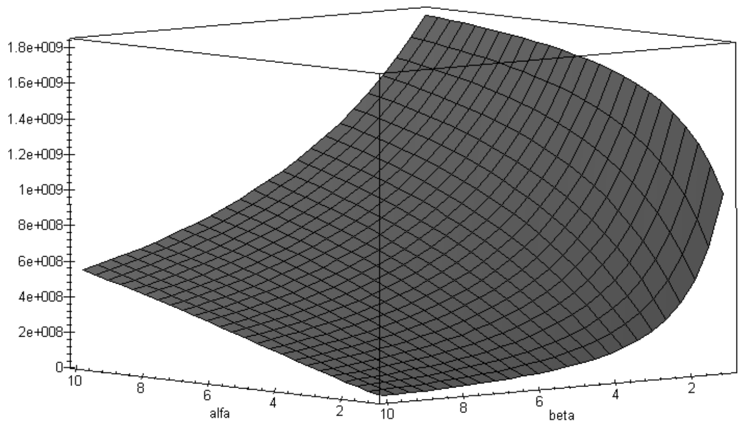

Figure 4.12. Parameter variability of $e^{(eff)}$ sensitivity gradient wrt parameter β

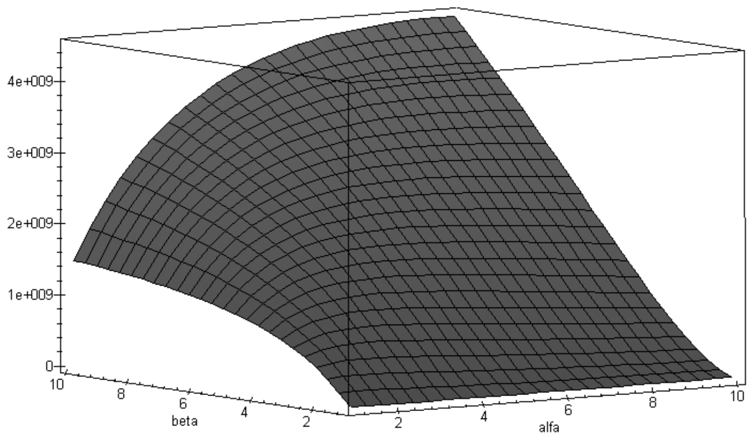

Figure 4.13. Parameter variability of $e^{(eff)}$ sensitivity gradient wrt parameter γ

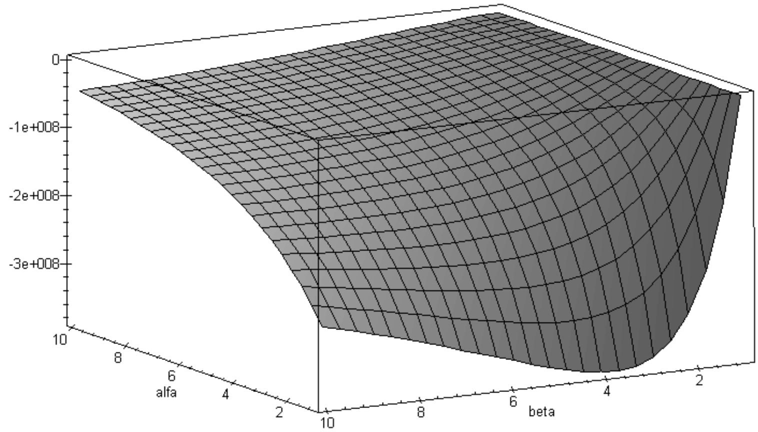

Figure 4.14. Second order sensitivity gradient of $e^{(eff)}$ wrt parameter α

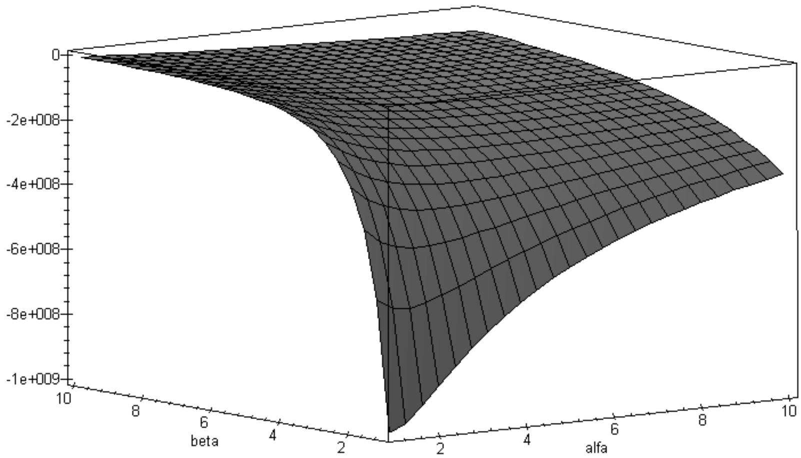

Figure 4.15. Second order sensitivity gradient of $e^{(eff)}$ wrt parameter β

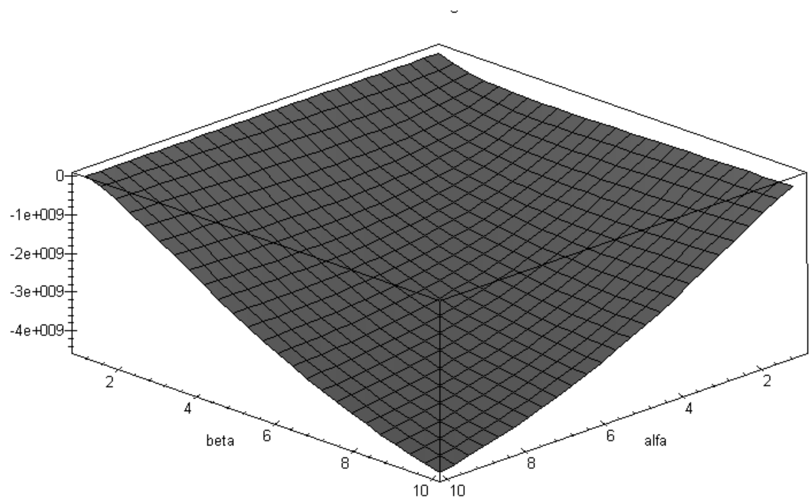

Figure 4.16. Second order sensitivity gradient of $e^{(eff)}$ wrt parameter γ

It is seen that in the case of both ratios equal to 1, the effective elasticity modulus is obtained as the value corresponding to a weaker material, which perfectly agrees with engineering intuition. Next, first and second order derivatives of the effective Young modulus of the composite with respect to the coefficients relating composite components are computed and analysed. It is typical that all the first order gradients are positive, while second order derivatives are less equal to 0. It reflects the fact that the overall effective Young modulus increase is obtained by the corresponding increase of any of these parameters. The second order sensitivity gradients computed and visualised above enable one to confirm the existence of an extremum of the first order derivatives presented before.

4.1.4 Material Sensitivity of Unidirectional Periodic Composites

The formulas describing the effective elasticity tensor components for the periodic composite with unidirectional distribution of the heterogeneities (see (2.103) – (2.107)) have been implemented in the symbolic computations package MAPLE to derive the appropriate sensitivity gradients [177]. The two−component composite shown schematically in Figure 4.17 was examined with the following input data for (a) weaker material e_2=4.0E9, ν_2=0.34, $c_2=1-c_1$ and (b) stronger material: e_1=4.0 E9 α, ν_1=0.34 β, c_1=0.5.

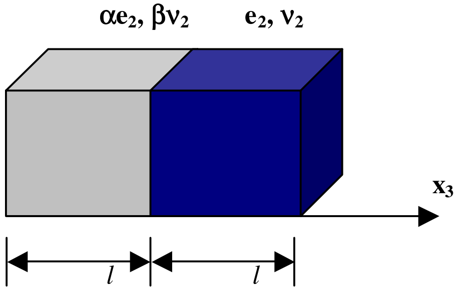

Figure 4.17. RVE of two−component composite bar

Design parameters α and β are introduced to make the visualisation of particular sensitivity gradients for some variations of the contrast between Young moduli and Poisson ratios of laminate layers. It will enable more successful optimisation of the composite in case of the homogenisation theory applications. The gradients collected on figures given below are normalised to make all the surfaces presented comparable to each other. First, quite obvious engineering interpretation of these results is that if particular gradient is less than 0 – an increase of design parameter accompanies a decrease of particular effective characteristic value. Otherwise (gradient greater than 0), an increase of the design parameter results in the appropriate increase of the homogenised quantity, while gradient comparable to 0 means that the given design parameter almost does not influence the overall effective characteristic. The figures plotted from the specially implemented MAPLE script present the sensitivity gradients of the homogenised elasticity tensor components – for $C^{(eff)}_{1111}$ (Figures 4.18−4.21), $C^{(eff)}_{3333}$ (Figures 4.22−4.25), $C^{(eff)}_{1133}$ (Figures 4.26−4.29), $C^{(eff)}_{1122}$ (Figures 4.30−4.33) and $C^{(eff)}_{1212}$ (Figures 4.34−4.37). Parameters α and β equivalent to the contrasts between stronger and weaker materials Young moduli and Poisson ratios are marked on the vertical axes of these figures, correspondingly.

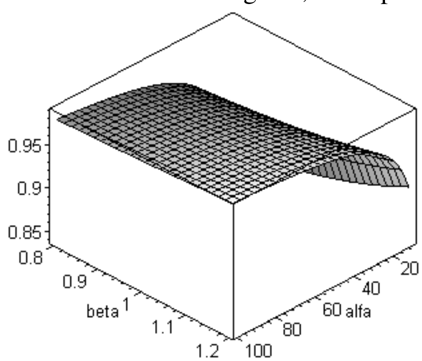

Figure 4.18. Sensitivity of $C^{(eff)}_{1111}$ wrt e_1

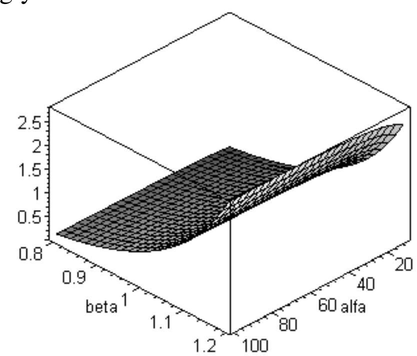

Figure 4.19. Sensitivity of $C^{(eff)}_{1111}$ wrt ν_1

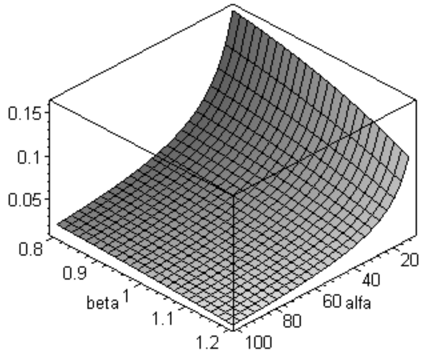

Figure 4.20. Sensitivity of $C^{(eff)}_{1111}$ wrt e_2

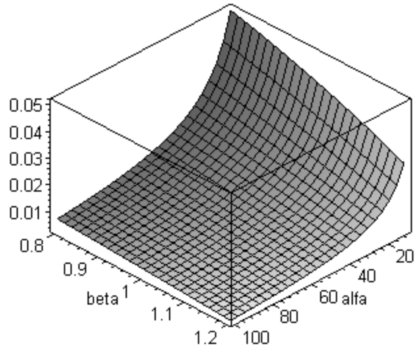

Figure 4.21. Sensitivity of $C^{(eff)}_{1111}$ wrt ν_2

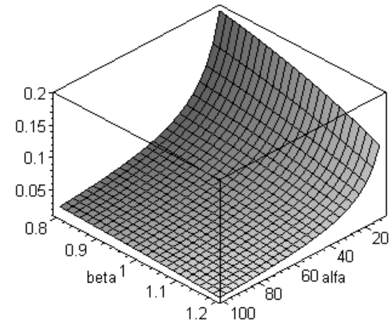

Figure 4.22. Sensitivity of $C^{(eff)}_{3333}$ wrt e_1

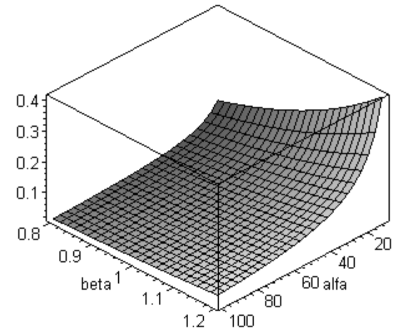

Figure 4.23. Sensitivity of $C^{(eff)}_{3333}$ wrt ν_1

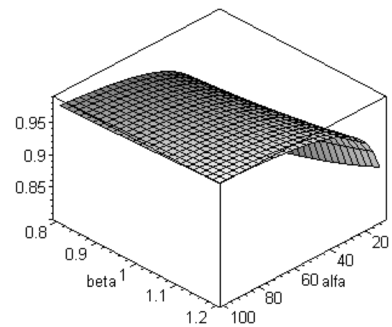

Figure 4.24. Sensitivity of $C^{(eff)}_{3333}$ wrt e_2

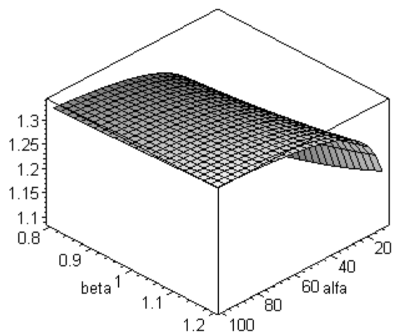

Figure 4.25. Sensitivity of $C^{(eff)}_{3333}$ wrt ν_2

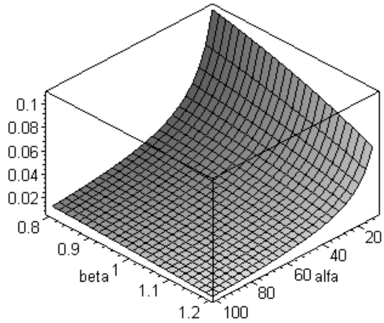

Figure 4.26. Sensitivity of $C^{(eff)}_{1133}$ wrt e_1

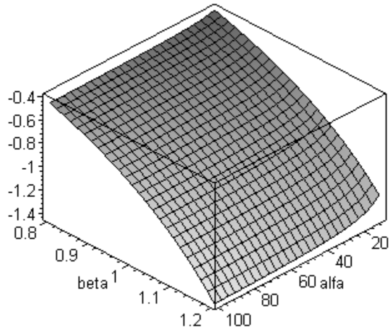

Figure 4.27. Sensitivity of $C^{(eff)}_{1133}$ wrt ν_1

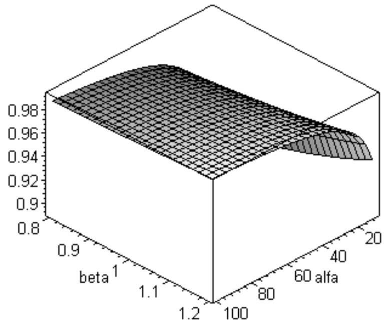

Figure 4.28. Sensitivity of $C^{(eff)}_{1133}$ wrt e_2

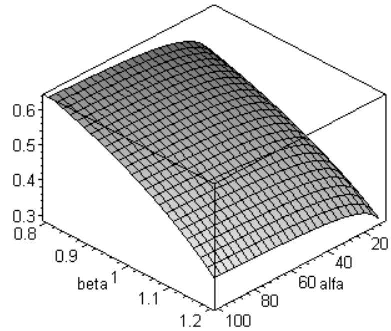

Figure 4.29. Sensitivity of $C^{(eff)}_{1133}$ wrt ν_2

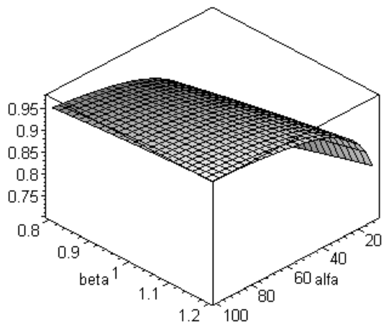

Figure 4.30. Sensitivity of $C^{(eff)}_{1122}$ wrt e_1

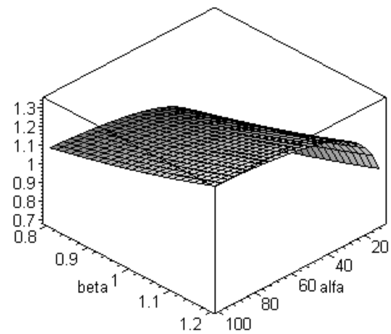

Figure 4.31. Sensitivity of $C^{(eff)}_{1122}$ wrt ν_1

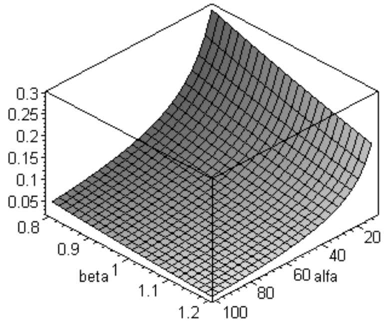

Figure 4.32. Sensitivity of $C_{1122}^{(eff)}$ wrt e_2

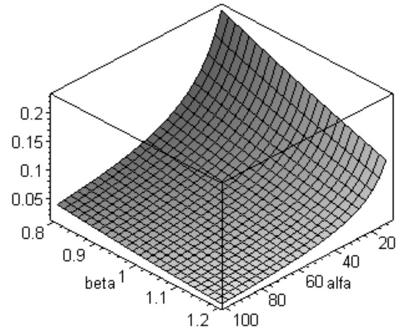

Figure 4.33. Sensitivity of $C_{1122}^{(eff)}$ wrt ν_2

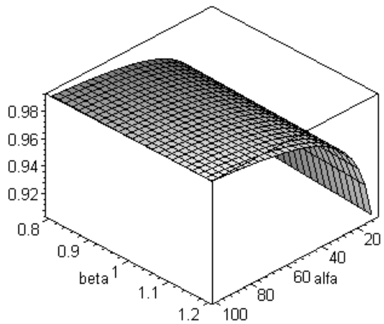

Figure 4.34. Sensitivity of $C_{1212}^{(eff)}$ wrt e_1

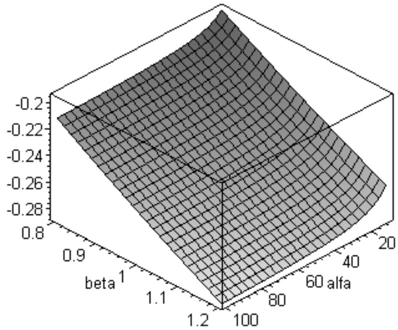

Figure 4.35. Sensitivity of $C_{1212}^{(eff)}$ wrt ν_1

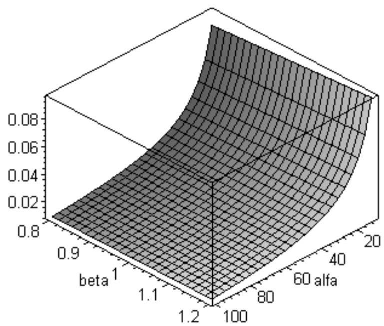

Figure 4.36. Sensitivity of $C_{1212}^{(eff)}$ wrt e_2

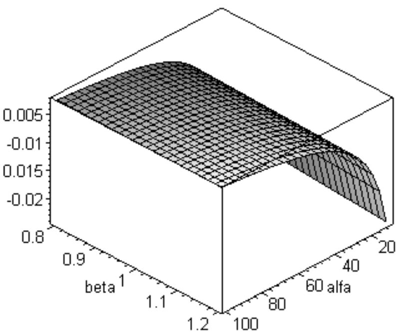

Figure 4.37. Sensitivity of $C_{1212}^{(eff)}$ wrt ν_2

How is demonstrated in all these figures, an increase of Young moduli of both stronger and weaker material result in the increase of all effective elasticity tensor components. Sensitivity gradients computed with respect to Poisson ratios of both composite components have mixed signs and all gradients essentially differ from 0. Taking into account particular variations and values of these results it can be observed that

(a) $C^{(eff)}_{1111}$ is sensitive at most wrt ν_1, then to e_1 and e_2 and at least to ν_2 and all gradients are positive;
(b) $C^{(eff)}_{3333}$ is most sensitive to ν_2, then to e_2, ν_1 and at least to e_1; all values are positive;
(c) $C^{(eff)}_{1133}$ is the most sensitive wrt e_2 and then to ν_2, e_1 and at least to ν_1 where the last parameter sensitivity analysis results in the negative gradient;
(d) $C^{(eff)}_{1122}$ (similarly to $C^{(eff)}_{1111}$) is most sensitive to ν_1, then to e_1 and e_2 and at least to ν_2 and all gradients have positive values;
(e) $C^{(eff)}_{1212}$ shows the greatest sensitivity wrt e_1, then to e_2 and finally to ν_2 and ν_1 where the last two variables give negative gradients.

Table 4.1. Sensitivity gradients for the unidirectional periodic composite

h	$\frac{\partial C^{(eff)}_{1111}}{\partial h}$	$\frac{\partial C^{(eff)}_{3333}}{\partial h}$	$\frac{\partial C^{(eff)}_{1133}}{\partial h}$	$\frac{\partial C^{(eff)}_{1122}}{\partial h}$	$\frac{\partial C^{(eff)}_{1212}}{\partial h}$	$G^{,h}$
e_1	0.9041	0.1138	0.0603	0.7696	0.9584	3.9570
e_2	0.0959	0.8862	0.9397	0.2304	0.0451	2.5430
ν_1	-0.0476	0.0368	-0.2811	0.7849	-0.1728	-1.1099
ν_2	0.0338	1.2018	0.6254	0.1891	-0.0105	1.8538

Furthermore, the sensitivity gradients of $G^{,h}$ with respect to all design parameters, i.e. Young moduli and Poisson ratios of both layers have been computed symbolically. They are found for equal values of components volume fractions in the RVE (50%) with the following material parameters: e_1=84.0 GPa, ν_1=0,22 and e_2=4.0 GPa, ν_2=0.34. All the gradients are collected in Tab. 4.1 – for particular components of the effective elasticity tensor and global composite structural response functional G. It is visible from these results that positive values of $G^{,h}$ are determined for e_1 and both material parameters of a weaker material, whereas negative – in case of stronger material Poisson coefficient. It should be mentioned that uniform strain field with $\varepsilon_{ij}=1$ is applied at the RVE to define this functional.

Particular values of the quantities $G^{,h}$ lead to the conclusion that the entire composite is the most sensitive with respect to Young modulus of stronger material, then to the parameters e_2 and ν_2 and at least – to the parameter ν_1. Comparing these results with analogous results obtained for the fibre−reinforced composite and collected in Tab. 2 it is observed that quite similar values are obtained in both cases and, moreover, both composites show negative sensitivity to Poisson ratios of stronger material. The fibre−reinforced composite is however the most sensitive with respect to the Poisson ratio of a composite weaker component.

Finally, is can be noted that since the procedure presented for unidirectional composite contains the algebraic approximations of homogenised characteristics depending on volume fractions of the components, the sensitivity gradients can be easily recalculated to include the volume fractions of both (or greater number of) constituents.

4.1.5 Sensitivity of Homogenised Properties for Fibre-Reinforced Periodic Composites

Material sensitivity of the periodic fibre−reinforced plane composite is studied here according to the numerical homogenisation method employed in Chapter 2. The sensitivity coefficients for effective elasticity tensor components with respect to the design parameters vector represented by **h** can be calculated using formula (2.131) as [167,177]

$$\frac{dC_{ijpq}^{(eff)}}{d\mathbf{h}} = \frac{\partial}{\partial \mathbf{h}}\left\{\frac{1}{|\Omega|}\int_{\Omega} C_{ijpq} d\Omega\right\} + \frac{\partial}{\partial \mathbf{h}}\left\{\frac{1}{|\Omega|}\int_{\Omega} C_{ijkl}\varepsilon_{kl}\left(\chi_{(pq)}\right) d\Omega\right\} \qquad (4.13)$$

which can be rewritten in the following form:

$$\frac{dC_{ijpq}^{(eff)}}{d\mathbf{h}} = \frac{1}{|\Omega|}\int_{\Omega}\frac{\partial C_{ijpq}}{\partial \mathbf{h}} d\Omega + \frac{1}{|\Omega|}\int_{\Omega}\frac{\partial C_{ijkl}}{\partial \mathbf{h}}\varepsilon_{kl}\left(\chi_{(pq)}\right) d\Omega + \frac{1}{|\Omega|}\int_{\Omega} C_{ijkl}\frac{\partial_{kl}\left(\chi_{(pq)}\right)}{\partial \mathbf{h}} d\Omega \qquad (4.14)$$

It is necessary to underline that differentiation with respect to any design sensitivity parameter can be inserted under the integration sign over the RVE, only if geometrical sensitivity with respect to composite composite dimensions is not accounted. It is observed that if the input sensitivity parameters are not the arguments of the elasticity tensor C_{ijkl}, the formula (4.14) simplifies to

$$\frac{dC_{ijpq}^{(eff)}}{d\mathbf{h}} = \frac{1}{|\Omega|}\int_{\Omega} C_{ijkl}\frac{\partial \varepsilon_{kl}\left(\chi_{(pq)}\right)}{\partial \mathbf{h}} d\Omega \qquad (4.15)$$

while the derivatives of the homogenisation functions $\chi_{(pq)}$ with respect to the components of vector h can be determined computationally by only. The first component of the sensitivity gradients in eqn (4.14) can be computed using analytical methods implemented in any symbolic computation packages. Furthermore, the sensitivity of $C_{ijpq}^{(eff)}$ components with respect to the fibre shape can be derived. However the final equations have a decisively more complicated form and they could be shown, only if the homogenisation function is derived analytically. Finally, the homogenised tensor derivatives are normalized as follows:

$$\left(\frac{dC_{ijpq}^{(eff)}}{d\mathbf{h}}\right)_{scaled} = \frac{\partial C_{ijpq}^{(eff)}}{\partial \mathbf{h}} \cdot \frac{h}{C_{ijpq}^{(eff)}(h)} \text{ (no summation over } i,j,p,q\text{)} \tag{4.16}$$

which makes it possible to compare all the homogenised tensor sensitivity gradients with each other and to establish quantitatively the most decisive parameters.

The most interesting problem however is not to determine the sensitivity coefficients of the homogenised tensor with respect to particular composite parameters but to approximate the sensitivity of the entire structure to its some design parameters. That is why, following previous considerations, we need to establish some structural response functional being an implicit function of the homogenisation function of the original composite design parameters [75,76,207,208]. This functional must represent the overall elastic strain (or complementary) energy for such a plane strain problem defined on the RVE which, after some minor modifications only, can be valid for numerous engineering applications in the composites engineering.

Therefore, let us define the sensitivity functional as the strain energy of the homogenised composite under a combination of the uniform constant strains in horizontal and vertical directions as well as for the transverse strain ε_{xy} as is illustrated below. In this case, the sensitivity functional can be expressed as

$$\begin{aligned} G &= \frac{1}{2}\int_{\Omega} \sigma_{ij}\varepsilon_{ij} d\Omega = \frac{1}{2}\int_{\Omega} \left(\sigma_{11}\varepsilon_{11} + \sigma_{12}\varepsilon_{12} + \sigma_{21}\varepsilon_{21} + \sigma_{22}\varepsilon_{22}\right) d\Omega \\ &= \frac{1}{2}\int_{\Omega} \left(\left\{C_{1111}^{(eff)}\varepsilon_{11} + C_{1122}^{(eff)}\varepsilon_{22}\right\}\varepsilon_{11} + \left\{C_{1212}^{(eff)}\varepsilon_{12} + C_{1221}^{(eff)}\varepsilon_{21}\right\}\varepsilon_{12}\right) d\Omega \\ &+ \frac{1}{2}\int_{\Omega} \left(\left\{C_{2121}^{(eff)}\varepsilon_{21} + C_{2112}^{(eff)}\varepsilon_{12}\right\}\varepsilon_{21} + \left\{C_{2211}^{(eff)}\varepsilon_{11} + C_{2222}^{(eff)}\varepsilon_{22}\right\}\varepsilon_{22}\right) d\Omega \end{aligned} \tag{4.17}$$

The strain state relevant to this functional can represent (a) uniaxial and/or biaxial compression/tension of the RVE; (b) shear (or torsion) of the composite specimen for ε_{11}=0 and ε_{22}=0 or (c) some combined strain state for the homogenised material.

Let us note that the difference between the vertical and horizontal strain tensor components is important in the case of an elliptical fibre and/or rectangular RVE where the extension of the cell give the unsymmetric strain field. Integrating over the RVE domain, recalling the assumed constant strain over this cell as well as a constant character of $C_{ijkl}^{(eff)}$ on Ω, one can get

$$G = \frac{l^2}{2}\left\{C_{1111}^{(eff)} + C_{1122}^{(eff)} + C_{1212}^{(eff)} + C_{1221}^{(eff)} + C_{2121}^{(eff)} + C_{2112}^{(eff)} + C_{2211}^{(eff)} + C_{2222}^{(eff)}\right\} \tag{4.18}$$

where l is a basic dimension of the RVE cell. Taking into account the elasticity tensor symmetry, the functional G can be expressed as

$$G = l^2\left\{C_{1111}^{(eff)} + C_{1122}^{(eff)} + 2C_{1212}^{(eff)}\right\} \tag{4.19}$$

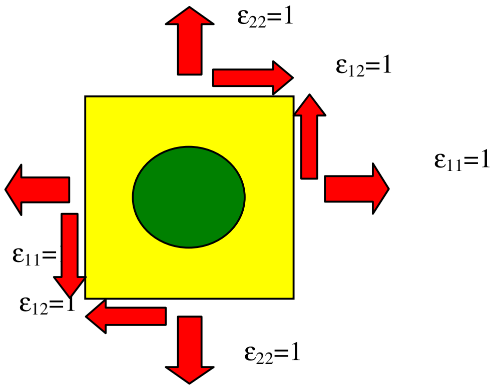

Figure 4.38. An idea of the structural response functional for the homogenised composite

Further, partial derivatives of G with respect to any component of the design parameters vector h can be calculated as

$$G^{,h} = \frac{\partial G}{\partial \mathbf{h}}$$
$$= \frac{\partial l^2}{\partial \mathbf{h}}\left\{C_{1111}^{(eff)} + C_{1122}^{(eff)} + 2C_{1212}^{(eff)}\right\} + l^2\left\{\frac{\partial C_{1111}^{(eff)}}{\partial \mathbf{h}} + \frac{\partial C_{1122}^{(eff)}}{\partial \mathbf{h}} + 2\frac{\partial C_{1212}^{(eff)}}{\partial \mathbf{h}}\right\} \tag{4.20}$$

The first component differs from 0 only if the design parameter vector contains the external diameter of the RVE. Otherwise, sensitivity gradients of this functional are determined as

$$G^{,h} = \frac{\partial G}{\partial \mathbf{h}} = l^2\left\{\frac{\partial C_{1111}^{(eff)}}{\partial \mathbf{h}} + \frac{\partial C_{1122}^{(eff)}}{\partial \mathbf{h}} + 2\frac{\partial C_{1212}^{(eff)}}{\partial \mathbf{h}}\right\} \tag{4.21}$$

Using this formula the most decisive design parameter for the homogenised composite in uniform plane strain can be determined having computed the effective elasticity tensor gradients from (4.13).

Finally, it is observed for the 1D heterogeneous structure with the constant cross−section A that the structural response functional G can be expressed as

$$G = \tfrac{1}{2}\int_{\Omega} \sigma\varepsilon d\Omega = \tfrac{A}{2}\int_{l} e^{(eff)}\varepsilon\varepsilon dy = \frac{Ae^{(eff)}}{2}\int_{l} \varepsilon^{2} dy \qquad (4.22)$$

which gives for the unit strain

$$G = \frac{Ae^{(eff)}l}{2} \qquad (4.23)$$

and then the sensitivity gradients of the functional G may be easily calculated by the chain rule as was proposed before.

The deterministic discretised homogenisation problem of elastic composites given by (4.14) is rewritten in the case of the DDM sensitivity studies as follows:

$$\frac{\partial K_{\alpha\beta}}{\partial \mathbf{h}} q_{(rs)\alpha} + K_{\alpha\beta}\frac{\partial q_{(rs)\alpha}}{\partial \mathbf{h}} = \frac{\partial Q_{(rs)\alpha}}{\partial \mathbf{h}} \qquad (4.24)$$

where the sensitivity gradients of homogenisation function components are calculated as

$$\frac{\partial q_{(rs)\alpha}}{\partial \mathbf{h}} = K_{\alpha\beta}^{-1}\left(\frac{\partial Q_{(rs)\alpha}}{\partial \mathbf{h}} - \frac{\partial K_{\alpha\beta}}{\partial \mathbf{h}} q_{(rs)\alpha}\right) \qquad (4.25)$$

If design variables are not the arguments of the RHS vector, it can be reduced to

$$\frac{\partial q_{(rs)\alpha}}{\partial \mathbf{h}} = -K_{\alpha\beta}^{-1}\frac{\partial K_{\alpha\beta}}{\partial \mathbf{h}} q_{(rs)\alpha} \qquad (4.26)$$

The derivatives of the stiffness matrix components $\frac{\partial K_{\alpha\beta}}{\partial \mathbf{h}}$ can be computed explicitly during the stiffness process formation or, alternatively, thanks to the finite difference scheme (FDM) presented below. Therefore, sensitivity coefficients of the effective elasticity tensor components are calculated starting from the above equations as

$$\frac{\partial C_{ijkl}^{(eff)}}{\partial \mathbf{h}} = \frac{1}{|\Omega|}\int_{\Omega} \frac{\partial C_{ijkl}}{\partial \mathbf{h}} d\Omega + \frac{1}{|\Omega|}\int_{\Omega} \frac{\partial C_{ijpq}}{\partial \mathbf{h}} B_{kl\gamma} q_{(pq)\gamma} d\Omega$$
$$+ \frac{1}{|\Omega|}\int_{\Omega} C_{ijkl} B_{kl\gamma} \frac{\partial q_{(pq)\gamma}}{\partial \mathbf{h}} d\Omega \tag{4.27}$$
$$= \frac{1}{|\Omega|}\int_{\Omega} \frac{\partial C_{ijkl}}{\partial \mathbf{h}} d\Omega + \frac{1}{|\Omega|}\int_{\Omega} \frac{\partial C_{ijpq}}{\partial \mathbf{h}} B_{kl\gamma} K_{\beta\gamma}^{-1} Q_{(pq)\beta} d\Omega$$
$$- \frac{1}{|\Omega|}\int_{\Omega} C_{ijkl} B_{kl\gamma} K_{\beta\gamma}^{-1} \frac{\partial K_{\beta\gamma}}{\partial \mathbf{h}} Q_{(pq)\beta} d\Omega + \frac{1}{|\Omega|}\int_{\Omega} C_{ijkl} B_{kl\gamma} K_{\beta\gamma}^{-1} \frac{\partial Q_{(pq)\beta}}{\partial \mathbf{h}} d\Omega$$

for $\alpha, \beta, \gamma = 1,..., N$. If, for example, the sensitivity parameter is introduced as the Young modulus $h \equiv e_a$, then the elasticity tensor is rearranged as

$$C_{ijkl}^{(a)}\left(e(\mathbf{x});\nu(\mathbf{x})\right) = e_a(\mathbf{x}) A_{ijkl}^{(a)}\left(\nu(\mathbf{x})\right) \tag{4.28}$$

and

$$\frac{\partial C_{ijkl}^{(a)}\left(e(\mathbf{x});\nu(\mathbf{x})\right)}{\partial e_a} = A_{ijkl}^{(a)}\left(\nu(\mathbf{x})\right) \tag{4.29}$$

while the finite element stiffness matrix component corresponding to *a*th material parameters can be expressed as

$$K_{\alpha\beta}^{(a)} = \int_{\Omega_a} C_{ijkl}^{(a)} B_{ij\alpha} B_{kl\beta} d\Omega = \int_{\Omega_a} e^{(a)} A_{ijkl}^{(a)} B_{ij\alpha} B_{kl\beta} d\Omega \tag{4.30}$$

As a result, the sensitivity of *m*th finite element stiffness matrix component with respect to the *a*th material Young modulus is computed as

$$\frac{\partial K_{\alpha\beta}^{(m)}}{\partial e^{(a)}} = \begin{cases} \int_{\Omega_a} A_{ijkl}^{(a)} B_{ij\alpha} B_{kl\beta} d\Omega; \ \mathbf{x}^{(m)} \in \Omega_a \\ 0; \ otherwise \end{cases} \tag{4.31}$$

Further, the sensitivity gradients of the RHS vector are obtained in a general form

$$\frac{\partial Q_{(pq)\alpha}}{\partial \mathbf{h}} = \frac{\partial \left(\left[C_{pq\alpha j}{}^{(a)}\right]\right) n_j}{\partial e_a} = \left[A_{pq\alpha j}{}^{(a)}\right] n_j \tag{4.32}$$

and the sensitivity of the effective elasticity tensor to Young modulus e_a is determined as

$$\begin{aligned}\frac{\partial C^{(eff)}_{ijkl}}{\partial e_a} &= \frac{1}{|\Omega|}\int_\Omega A^{(a)}_{ijkl}\, d\Omega + \frac{1}{|\Omega|}\int_\Omega A^{(a)}_{ijkl} B_{ij\gamma} K^{-1}_{\gamma\beta} Q_{(pq)\beta}\, d\Omega \\ &+ \frac{1}{|\Omega|}\int_\Omega C^{(a)}_{ijkl} B_{ij\gamma}\left[\sum_{a=1}^{E}\int_{\Omega_a} A^{(a)}_{ijkl} B_{ij\gamma} B_{kl\beta}\, d\Omega\right] Q_{(pq)\beta}\, d\Omega \\ &+ \frac{1}{|\Omega|}\int_\Omega C^{(a)}_{ijkl} B_{ij\gamma} K^{-1}_{\beta\gamma}\left[A^{(a)}_{pq\beta j}\right] n_j\, d\Omega\end{aligned} \tag{4.33}$$

Analogously, the sensitivity gradients of the effective elasticity tensor components for a composite with respect to the Poisson ratios can be calculated but since the elasticity tensor is a complex function of these ratios, the derivation is omitted here.

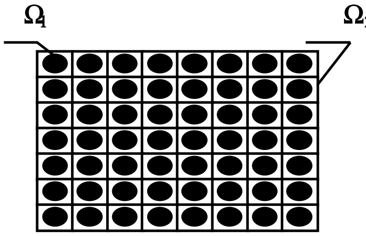

Figure 4.39. Periodic composite specimen

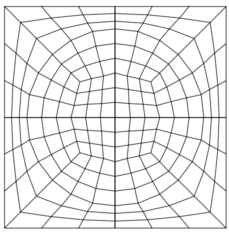

Figure 4.40. Mesh of the periodicity cell

Let us consider for illustration the composite with periodicity cell shown in Figure 4.39 – the fibre has a round cross–section and the entire RVE is rectangular. The analysed composite is assumed to be perfectly periodic with fibres distributed uniformly in the transverse cross–section, while the reinforcement ratio is equal to 50% of the total area of the RVE. Material characteristics for the computational analysis are taken as follows: e_1=84.0 GPa, e_2=4.0 GPa, ν_1=0.34 and ν_2=0.22; the FEM discretisation using 4-node linear plane strain elements is presented in Figure 4.40.

Computational sensitivity studies are carried out to determine the sensitivity gradients of the effective elasticity tensor components with respect to material parameters of the constituents, i.e. Young moduli and Poisson ratios of fibre and matrix. All computational tests are done by the use of the specially tailored computer program MCCEFF [167,173], designed and implemented for deterministic and stochastic computational homogenisation−based studies. The variability of the sensitivity gradients of the effective elasticity tensor components resulting from the perturbation parameter variations are presented in Figures 4.41 – 4.52: for the component $C_{1111}^{(eff)}$ (Figures 4.41−4.44), for the component $C_{1122}^{(eff)}$ (Figures 4.45−4.48), and for $C_{1122}^{(eff)}$ in Figures 4.49−4.52. The sensitivity gradients are marked on the horizontal axes for three different ranges of parameter increments shown on the vertical axes. These series correspond to the homogenised tensor increments in the range of promiles (O(-3)), percents (O(-2)) and tenths (O(-1)) of the verified parameter. The numerous experiments result from the fact that, as was expected and shown numerically, particular values of sensitivity gradients of the effective tensor components depend on the perturbation of a given material parameter employed as the design parameter.

Table 4.2. Sensitivity gradients of the effective elasticity tensor

h	$\frac{\partial C_{1111}^{(eff)}}{\partial h}$	$\frac{\partial C_{1122}^{(eff)}}{\partial h}$	$\frac{\partial C_{1212}^{(eff)}}{\partial h}$	$G^{.h}$
e_1	0.141	0.072	0.958	2.129
v_1	0.056	0.180	-0.173	-0.090
e_2	0.867	0.926	0.044	1.881
v_2	1.205	2.814	-0.011	3.987

As can be observed on all these graphs, the worst numerical stability of sensitivity gradients is obtained for the smallest perturbation order O(-3) and can result from the computational error of the homogenisation method itself. This numerical phenomenon can be studied in terms of the discretisation density of the RVE in the homogenisation analysis and with respect to the reinforcement ratio of the entire composite. Another phenomenon, resulting from physical aspects of the composite being visible especially in Figures 4.44, 4.48 and 4.52 in the case of the sensitivities of O(-1) order, is caused by the fact that the Poisson ratio of the matrix tends to its upper physical limit for this variable, which results in an uncontrolled increase of the components $C_{1111}^{(eff)}$ and $C_{1122}^{(eff)}$ sensitivity gradients. Because of that, greater values of $C_{ijkl}^{(eff)}$ derivatives with respect to $\Delta\nu_2$ do not exist.

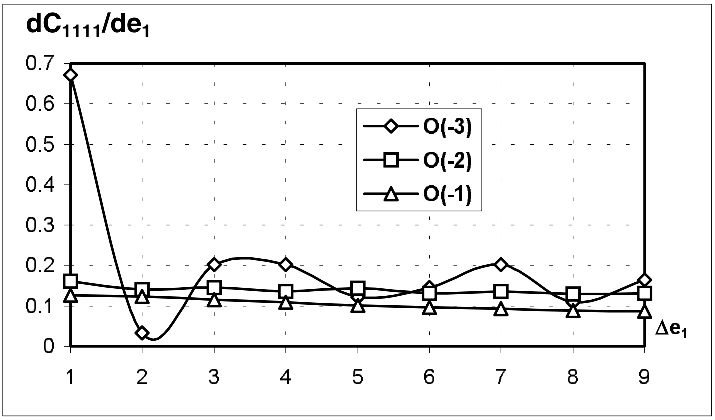

Figure 4.41. Sensitivity of $C_{1111}^{(eff)}$ wrt e_1

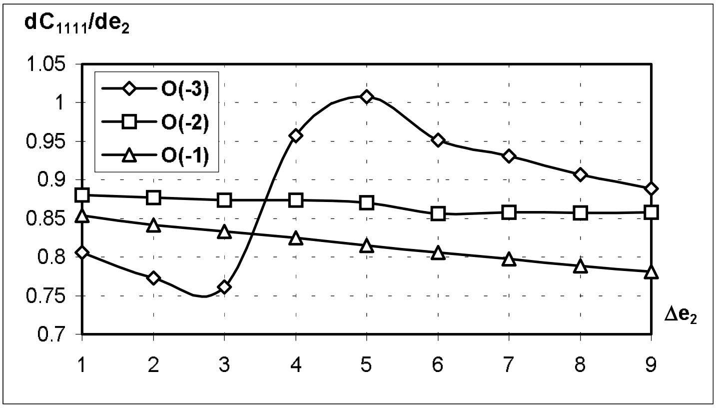

Figure 4.42. Sensitivity of $C_{1111}^{(eff)}$ wrt e_2

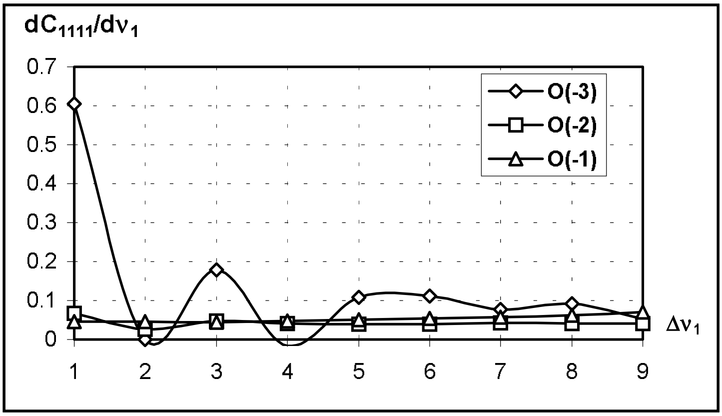

Figure 4.43. Sensitivity of $C_{1111}^{(eff)}$ wrt ν_1

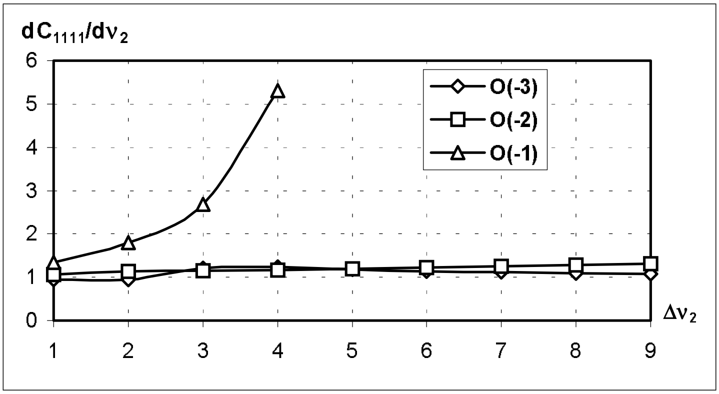

Figure 4.44. Sensitivity of $C_{1111}^{(eff)}$ wrt ν_2

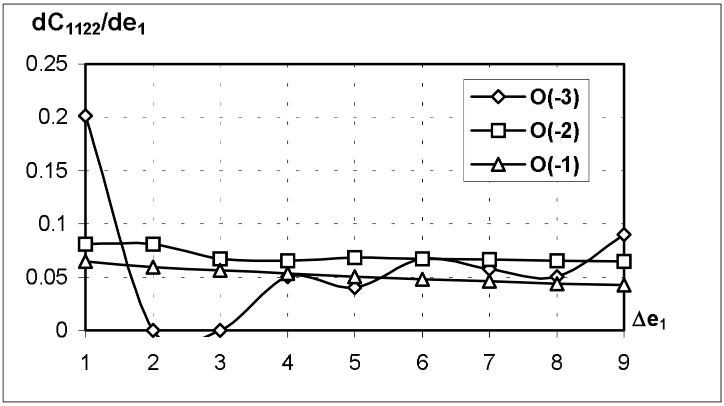

Figure 4.45. Sensitivity of $C_{1122}^{(eff)}$ wrt e_1

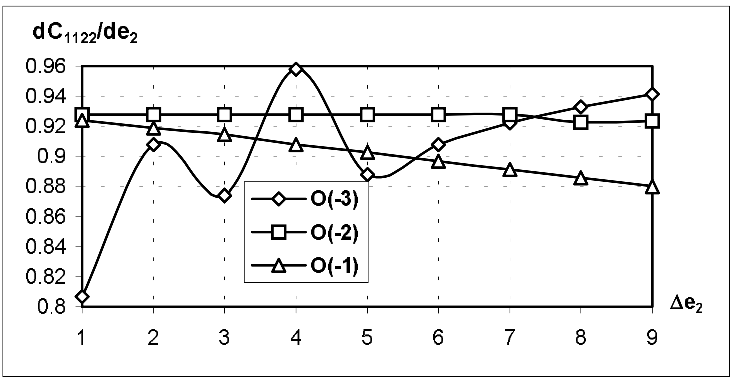

Figure 4.46. Sensitivity of $C_{1122}^{(eff)}$ wrt e_2

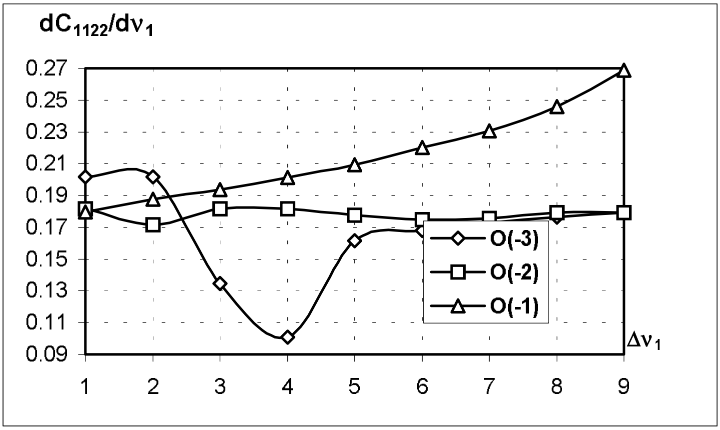

Figure 4.47. Sensitivity of $C_{1122}^{(eff)}$ wrt ν_1

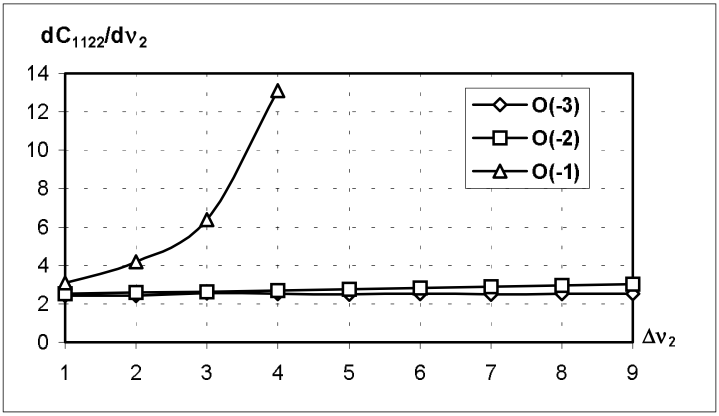

Figure 4.48. Sensitivity of $C_{1122}^{(eff)}$ wrt ν_2

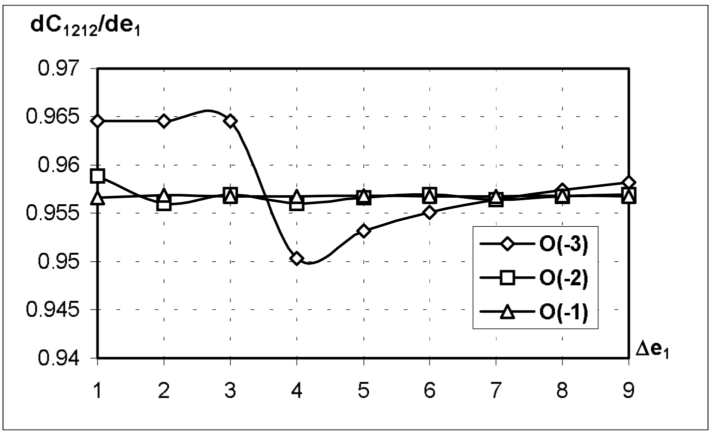

Figure 4.49. Sensitivity of $C_{1212}^{(eff)}$ wrt e_1

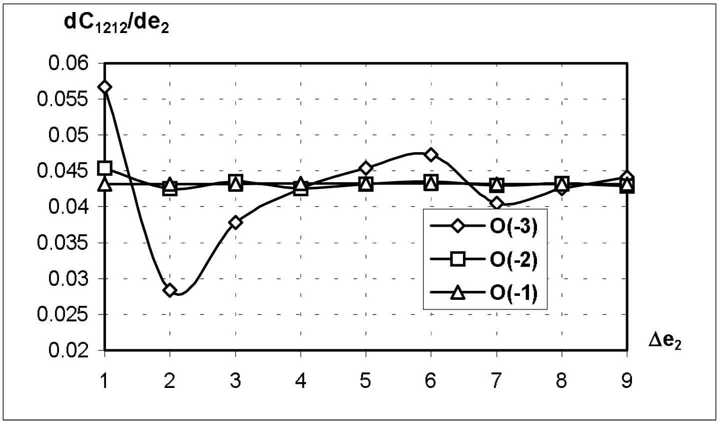

Figure 4.50. Sensitivity of $C_{1212}^{(eff)}$ wrt e_2

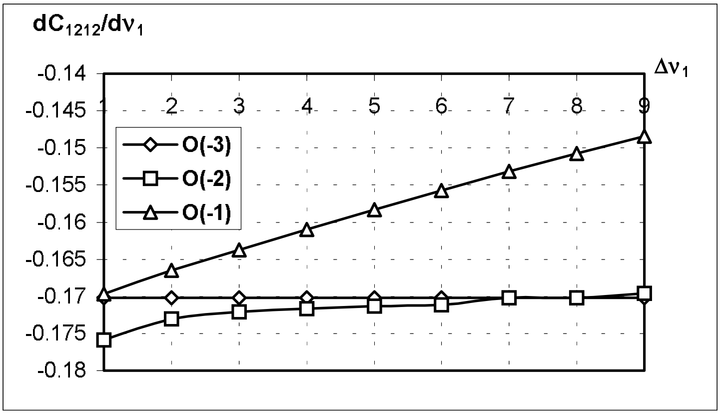

Figure 4.51. Sensitivity of $C_{1212}^{(eff)}$ wrt ν_1

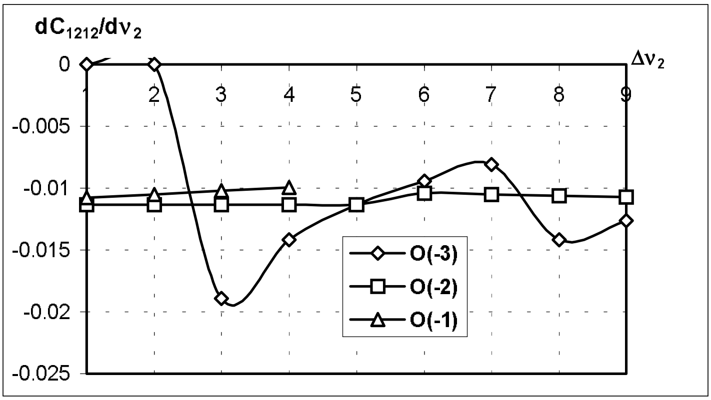

Figure 4.52. Sensitivity of $C_{1212}^{(eff)}$ wrt ν_2

Next, comparing all the figures, it is seen that the best numerical stability is obtained for the computational series corresponding to O(-2). The sensitivity gradients in this range are almost constant for 1−10% of all input parameters perturbations. Starting from these results, a more detailed comparison, both from a computational and engineering point of view, can be carried out for various FEM mesh sizes and the interrelations of design parameter mean values. It should be noticed that, as for the 1D composite example, a negative sign of the sensitivity gradient is equivalent to a decrease of a particular $C_{ijkl}^{(eff)}$ component, accompanying the increase of this parameter value; a positive derivative corresponds to the opposite relation.

Observing the particular results of computational analysis it can be noticed that most sensitivity gradients are positive (except those shown in Figures 4.51 and 4.52), which basically means that an increase of most elastic characteristics of fibre−reinforced composite components results in corresponding increase of the overall effective elasticity tensor; the effective elasticity tensor components $C_{1111}^{(eff)}$ and $C_{1122}^{(eff)}$ are sensitive at most to Poisson ratios of the composite constituents. The component $C_{1212}^{(eff)}$ is sensitive to the Young modulus of the matrix (with a negative sign). Furthermore, it is seen that particular values of the presented gradients depend strongly on the interrelations between the main values of Young moduli and Poisson ratios of the entire structure. That is why the observed phenomena are the best illustration of the material sensitivity of glass−epoxy periodic composites only. The results collected in Table 4.2 can be compared against those obtained before for essentially different interrelations between the composite components – we observe in that study that for similar constituents the signs of particular gradients are exactly the same. However the values are qualitatively different. This is why such an analysis must be oriented to the particular composite; otherwise it should be carried out for the very particular engineering application of the analysed composite.

The sensitivity with respect to the reinforcement shape, local lack of periodicity as well as material parameters in the case of inelastic behaviour of the constituents may be verified numerically in further computational studies on homogenised properties of the composites. On the other hand, it seems to be reasonable to verify the computed sensitivity gradient to the interrelation between corresponding elastic properties of the components (the ratio of Young modulus in a fibre to Young modulus of a matrix, for instance). This study would validate if all groups of various composites with the same geometry of the RVE had the same or at least comparable sensitivity gradients.

Finally, the approximation of the determined gradients by some specific values is proposed and, considering all the remarks posed above, it is established as the arithmetic average of the gradients corresponding to 1% and 10% increments of the design parameters. These values are used to approximate the value of $G^{,h}$ computed on the basis of (4.21), which are scaled over the RVE total area. Using such a composite structure response functional, the Poisson ratio of a matrix and the next Young modulus of the fibre are detected as the most decisive design material parameters of this composite in the view of its homogenised elastic parameters.

4.2 Probabilistic Analysis

The main purpose of the sensitivity analysis is to verify numerically the influence of some particular input parameters on the analysed state functions. In the case of the homogenisation procedure, the sensitivity of the effective elasticity tensor can be verified in terms of material parameters of the constituents, reinforcement shape and its spatial distribution, the volume ratios of the components, etc.; material parameters of composite constituents are taken below as design parameters.

Analogous situation takes place in case of probabilistic analysis, however the total number of possible design parameters dramatically increases. It reflects the fact that each geometrical and material parameter is usually represented by its at least two probabilistic moments. Hence, all probabilistic moments of all input variables can be considered as design parameters. At the same time, the sensitivity gradients can be computed in addition to any probabilistic moment of the state function determined during a structural modeling. Therefore, we can determine the sensitivity gradients of expected values of displacement vector to the expected values and/or standard deviations of structural members thickness, length or elastic parameters. Similarly, the cross-correlation function or standard deviation of the resulting state variables can be the subject of the SDS analysis.

Using the definition of effective elasticity tensor, the sensitivity of the *m*th order probabilistic moment of this tensor with respect to the *n*th order central probabilistic moment of an input random design variable vector **h** can be formulated as

$$\frac{\partial\left(\mu_m\left(C_{ijkl}^{(eff)}(\mathbf{h};\omega)\right)\right)}{\partial\mu_n(\mathbf{h})}=\frac{\partial}{\partial\mu_n(\mathbf{h})}\left(\mu_m\left(\int_\Omega C_{ijkl}(\mathbf{h};\mathbf{x};\omega)d\Omega\right)\right)$$
$$+\frac{\partial}{\partial\mu_n(\mathbf{h})}\left(\mu_m\left(\int_\Omega \sigma_{ij}\left(\chi^{(kl)}(\mathbf{h};\mathbf{x};\omega)\right)d\Omega\right)\right) \tag{4.34}$$

The first component of the RHS summation can be derived analytically or symbolically, whereas the second one can be obtained numerically only by using the Finite or Boundary Element Method programs adopted for any probabilistic technique. If the effective material tensor is represented by the closed form function of the elastic properties of composite components, then it is possible to derive analytically probabilistic moments of a homogenised tensor. Alternatively, the Monte Carlo simulation technique may be used to randomise and estimate the sensitivity gradients of any order probabilistic moments with respect to the effective elasticity tensor components.

Numerical illustration is carried out by an application of the Monte Carlo simulation for a homogenisation cell problem have been performed using specially modified FEM code MCCEFF and its 4−node rectangular isoparametric plane strain finite elements. The results of computations are expected now as the partial derivatives of probabilistic moments of the effective elasticity tensor with respect to relevant probabilistic moments of elastic or geometrical characteristics of the fibre and/or matrix as well as the interface defects (Young modulus of the matrix is treated here as the design probabilistic variable).

Sensitivity gradients of up to the fourth order probabilistic characteristics of the homogenised elasticity tensor components with respect to $\mathbf{h} \equiv e_2(\omega)$ being uncorrelated Gaussian random variables are obtained for the following data: $E[e_1]=84.0\,E6$, $E[e_2]=4.0\,E6$, $Var(e_1)=70.56\,E12$, $Var(e_2)=16.0\,E10$; it corresponds to the coefficient of variation equal to 0.1 for both Young moduli. The interface defects (model with 'bubbles') are simulated numerically in such a way that a 10% elastic characteristic reduction in the interphase is obtained and they are compared against the results computed for a composite with perfectly bonded components (model with 'no bubbles'). The results of simulations are collected in Table 4.3 as sensitivity gradients of first two probabilistic moments of the homogenised elasticity tensor components with respect to expected value and the variance of the matrix Young modulus.

Table 5.3. Probabilistic sensitivity gradients of the homogenised elasticity tensor

Probabilistic moment	$\frac{\partial}{\partial E[e_2]}$		$\frac{\partial}{\partial Var(e_2)}$	
	'Bubbles'	'No bubbles'	'Bubbles'	'No bubbles'
$E[C_{1111}^{(eff)}]$	0.0819	0.0817	-0.0001	-0.0001
$\alpha(C_{1111}^{(eff)})$	-0.0748	-0.0747	0.0405	0.0405
$\beta(C_{1111}^{(eff)})$	-0.0076	-0.0127	-0.0005	-0.0064
$\gamma(C_{1111}^{(eff)})$	-0.0003	0.0005	-0.0004	0.0000
$E[C_{1122}^{(eff)}]$	0.0892	0.0893	-0.0001	-0.0001
$\alpha(C_{1122}^{(eff)})$	-0.0815	-0.0815	0.0438	0.0438
$\beta(C_{1122}^{(eff)})$	0.0082	0.0059	0.0012	0.0013
$\gamma(C_{1122}^{(eff)})$	0.0003	0.0002	0.0002	0.0003
$E[C_{1212}^{(eff)}]$	0.0043	0.0043	-0.00006	0.0000
$\alpha(C_{1212}^{(eff)})$	-0.0043	-0.0043	0.0020	0.0020
$\beta(C_{1212}^{(eff)})$	0.0000	-0.0001	0.0003	-0.00002
$\gamma(C_{1212}^{(eff)})$	0.0000	0.0000	0.0000	0.0000

The results collected above show that the most sensitive probabilistic moment of the homogenised tensor component with respect to $E[e_2]$ is the expected value of $E[C_{1122}^{(eff)}]$, which is slightly greater than the result computed for $E[C_{1111}^{(eff)}]$. An analogous relation is observed in addition to the coefficient of variation $\alpha(C_{1122}^{(eff)})$ and $Var(e_2)$. However sensitivity gradients determined with respect to the expected value are significantly greater than those obtained for the variance, which partially reflects the input coefficient of the variation of the matrix Young modulus. The smallest sensitivity of random variable $C_{1212}^{(eff)}(\omega)$ with respect to the random input $e_2(\omega)$ is observed also, while the fourth order coefficients of concentration are in practice neither sensitive to $E[e_2]$ nor to $Var(e_2)$, which follows the Gaussian type of both input and output probabilistic distributions in homogenisation problems. The most sensitive statistical estimator is the coefficient of asymmetry – some differences are observed between the models with and without interface bubbles, where some sign changes are also noticeable.

Comparing the probabilistic gradients computed for the composite with and without the interphase some small variations between these two models are observed. These variations however can increase together with further weakening of the interphase and detailed computer simulation can verify this tendency.

Further computations are necessary to study the variability of the obtained results with respect to the chosen increment during the numerical differentiation process; the proposed value of 10% has been detected as the most effective in previous computations. An increase in effectiveness of the numerical procedure can be achieved by implementation of a semi−analytical homogenisation procedure, where the sensitivity gradients of spatially averaged effective elasticity tensor components are determined symbolically using the system MAPLE, for instance, and an averaged stress tensor is differentiated numerically using the finite difference scheme.

4.3 Conclusions

The sensitivity analysis of homogenised material tensors, proposed and carried out in this Chapter, makes it possible to consider the influence of particular material parameters of the composite components on the overall effective properties of a composite. Thanks to such an analysis, a composite designer can generally determine the most decisive material characteristics of the constituents (Poisson ratios of fibre and matrix for a 2D composite, for instance) and then, modifying their values during the design process, can optimise the composite structure for the effective parameters given *a priori*. The sensitivity equations for homogenisation of linear elastic composites can be extended to an analogous analysis for effective properties of composites with viscoelastoplastic components, both in a deterministic and probabilistic context. The proposed methodology has a general character, however further examination of various composites (beams, plates, 2D and 3D structures) should give different results.

Particular computational studies, performed in terms of perturbation parameter ε applied in sensitivity gradients analysis, show that the best numerical stability is obtained for $\varepsilon \approx O(-2)$. Smaller order taken in numerical analysis causes significantly greater deviations of the final result, while the lack of physical sense of the problem is obtained for $\varepsilon \approx O(-1)$, where the Poisson ratio is taken as a design parameter. Further computations should be carried out to determine the RVE mesh and the finite element type influence on the final result.

Considering the assumption that the scale factor between the periodicity cell and the entire composite structure tends to 0 and, on the other hand, that this quantity in real composites is small and positive, but differs from 0, the sensitivity of the effective characteristics for this parameter is to be calculated next using the so-called homogenisation micro−macro analysis, for instance. To make such an analysis, the scale parameter must be inserted in equations describing the effective quantities and then, the influence of the relation between the micro− and macrostructure must be shown.

Sensitivity analysis of the 1D, 2D and 3D homogenisation of effective heat conductivity carried out in this chapter may be applied for any linear potential field problem − irrotational and incompressible fluid flow, film lubrication, acoustic vibration as well as for electric conduction, electrostatic field and electromagnetic waves. To use these results for homogenisation of other engineering problems, the well−known field analogies may be applied to transform the effective Young modulus to related physical field parameters.

Proposed methodology of the sensitivity gradient computations for homogenised tensor components of periodic random composites is exact in the probabilistic sense because of the application of the Monte Carlo simulation technique. The use of the MCS technique preserves the existence and uniqueness of the classical homogenisation problem solution – it exists for each realisation separately. Therefore, thanks to the statistical estimation implementation, a mathematically correct probabilistic characterisation of the homogenised tensor components is obtained. The numerical weakness of the finite difference apparatus implemented in the homogenisation−oriented FEM code should be eliminated in further simulations by the verification of the sensitivity gradient values with respect to variations of the input parameter increments. As is documented by some previous computations, lack of numerical stability of such sensitivity computations is observed for physical parameters tending to their physical bounds.

An analogous procedure can be applied to determine the sensitivity gradients of homogenised characteristics of other composites, i.e. 1D periodic beams, plates, shells, periodic 3D structures with particles and fibres of various shapes as well as multi–component engineering structures as superconducting devices [168] studied before. A linear elastic model in sensitivity analysis may be extended to inelastic homogenised characteristics [118,230,307] as well as on stochastic optimisation of composites through the homogenisation method.