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# Thermal stresses in a coating layer. I. General theoretical scheme

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**Abstract** The evolution of thermal stresses generated by a thermal perturbation of cylindrical symmetry in a flat infinite isotropic thermoelastic layer of constant (before perturbation) thickness on a half-space rigid substrate is theoretically investigated. The problem is considered in the framework of uncoupled linear thermoelasticity, in the quasi-stationary displacement field approximation. Thermal insulation of the layer is considered in two versions: (a) both its surfaces are adiabatically insulated, and (b) the free surface is adiabatically insulated, whereas the contact surface is kept at constant temperature. The free surface of the layer is assumed to be stress free, and the contact surface is kept on a rigid substrate. The proper equations are solved using suitable Hankel and Fourier transformations. Part I of the paper presents a general theoretical scheme of the problem in a general case (without specification of the perturbation), and it is illustrated by a simple, detailed example (time evolution of stresses at the contact surface of the layer, generated by a surface point instantaneous heat pulse in case a). The analysis of stresses in more realistic cases, modeling realistic situations will be presented in Part II.

## 1 Introduction

The evolution of a stress field generated in a layer by heat perturbation may be important, among others, for stability and life of coating layers.<sup>1</sup> If perturbation is sufficiently strong and it amplifies residual stresses in the system, then the total stresses can achieve levels which may be dangerous for the compressing strength (or tensile strength, depending on the sign of thermal stresses) for the coating material, or for the cohesive strength of the connection of the coating with the substrate. Thermal stresses in coating layers have rich literature concerning various particular cases and aspects (see for example [2–12]). A general approach to the analysis of thermal stresses in thin layers generated by a thermal loading was initiated, among others, by Rudin under some simplifying assumptions [13], and next elaborated by Elperin and Rudin in a more general version [14]. However, the Elperin–Rudin scheme leads to surprising conclusions that—first—the normal stress at the interface vanishes, and—second—in a particular case of a homogeneous layer on a rigid isothermal substrate

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<sup>1</sup> Laser heat perturbation is used for testing the thermal reliability of coatings in the so called laser thermal shock method (see for example [1]).

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also the tangent stress at the interface vanishes.<sup>2</sup> Therefore, it seems that the general theory of thermal stresses in coating layers generated by a heat loading is still waiting for further elaboration. We start here with the simplest model, namely a homogeneous coating layer on a rigid substrate.

## 2 Statement of the problem

A theoretical analysis of thermal stresses in a coating layer is performed using the following model, thought as representing typical realistic situations. The coating is assumed to be an infinite flat layer of constant (before thermal perturbation) thickness on a half-space rigid substrate. No external forces act on the layer. The coating substance is assumed to be an isotropic linear thermoelastic material [i.e. the thermal equation of state for the material is given by the Duhamel–Neumann equation in the approximation of small deformation and with constant material parameters—see below, Eqs. (2.1.3–5)]. The analysis is performed (i) in the framework of uncoupled linear thermoelasticity (the influence of mechanical phenomena on heat conduction is neglected, i.e. the heat conduction equation does not contain the coupling term, and all the material parameters, including density, are constants), and (ii) in the quasi-stationary displacement field approximation (i.e. the acceleration term in the equation of motion is neglected). The latter assumption means that the analysis is limited to quasi-static mechanical effects of the thermal perturbation, which usually takes place in realistic situations with not very rapid thermal perturbation (for detail criteria of these assumptions see [15]).

Thus, the governing equations are (see [16])

$$\rho c \frac{\partial T}{\partial t} = \lambda \nabla^2 T + q, \quad (2.1.1)$$

$$(1 - 2\nu) \nabla^2 u + \nabla(\nabla \cdot u) = 2(1 + \nu) \alpha \nabla T, \quad (2.1.2)$$

$$\sigma = \frac{E}{(1 + \nu)(1 - 2\nu)} [(1 - 2\nu)\varepsilon + \nu I Tr(\varepsilon) - (1 + \nu)\alpha IT], \quad (2.1.3)$$

$$\varepsilon = \frac{1}{2} [\nabla u + (\nabla u)^T], \quad Tr(\varepsilon) = \nabla \cdot u, \quad (2.1.4)$$

where  $t$  stands for time,  $T$ —for temperature [counted from the homogeneous initial (before perturbation) value],  $q$ —for heat source (and represents the thermal perturbation);  $\rho$ ,  $c$  and  $\lambda$ —for density, specific heat and heat conductivity, respectively;  $u$ ,  $\sigma$  and  $\varepsilon$ —for displacement vector, stress tensor and strain tensor, respectively;  $\nabla$ —for nabla operator,  $I$ —for unit tensor of second order;  $()^T$ —for transposed tensor;  $E$ ,  $\nu$  and  $\alpha$ —for Young's modulus, Poisson's coefficient and (linear) heat expansion coefficient, respectively.

In the initial state (before perturbation), the layer is assumed to be homogeneous and in full equilibrium (both thermal and mechanical). The thermal insulation of the layer is assumed in two alternative versions representing extreme cases of realistic situations, namely: (case *a*) both surfaces are insulated adiabatically (as a model of the substrate material being a good thermal insulator when compared to the coating material), or (case *b*) the external surface of the coating material is adiabatically insulated, and the internal surface (the surface of the contact of the coating layer and the substrate material) is kept at temperature equal to zero (as a model of the substrate material being a good thermal conductor when compared to the coating material). The layer is assumed to be unbounded, i.e. it is stress free on the free surface, and it is unmovable on the surface of its contact with the substrate.

The perturbation term  $q$  will be specified in detail later while modeling realistic situation. At the beginning, it is assumed only to be (spatially) localized and to possess cylindrical symmetry.

The cylindrical symmetry is also assumed for the boundary conditions, so each of the considered detailed problems is cylindrically symmetrical, and therefore will be formulated and solved in the cylindrical coordinate system  $r$ ,  $\varphi$ ,  $z$  with the  $z$ -axis directed perpendicularly from the free coating surface toward the substrate material. All the fields are independent of the azimuth coordinate  $\varphi$  by the assumed symmetry.

The structure of the set represented by Eq. (2.1) suggests the following procedure for realizing the program:

- (i) solve the heat conduction equation,
- (ii) solve the equation for displacement field,
- (iii) calculate strain field,
- (iv) calculate and analyse the stress field.

<sup>2</sup> As will be seen later in our paper, these conclusions are not confirmed in the scheme presented here.

This program will be realized in Part I almost in full in general version, i.e. without specification of heat perturbation (heat source term in heat conduction equation). An analysis of the stress field will be presented in Part II for cases of specified thermal perturbations, modeling realistic situations. Here only a simple illustrative example will be given. Before we start to realize the program we introduce dimensionless variables.

### 3 Dimensionless variables

All the introduced dimensionless variables will be denoted in this Section by a bar. We introduce the following dimensionless independent variables:

$$\bar{r} := \frac{r}{h}, \quad \bar{z} := \frac{z}{h}, \quad \bar{t} := \frac{\kappa}{h^2}t, \quad (3.1)$$

where  $h$  stands for layer thickness (before perturbation), and  $\kappa = \lambda/(\rho c)$  for temperature conductivity (heat diffusivity).

The functions  $T, q, u, \sigma$  and  $\varepsilon$  are referred to their characteristic values  $T_c, q_c, u_c, \sigma_c$  and  $\varepsilon_c$ ,

$$\bar{T} = \frac{T}{T_c}, \quad \bar{q} = \frac{q}{q_c}, \quad \bar{u} = \frac{u}{u_c}, \quad \bar{\sigma} = \frac{\sigma}{\sigma_c}, \quad \bar{\varepsilon} = \frac{\varepsilon}{\varepsilon_c}, \quad (3.2)$$

where

$$T_c = \frac{h^2 q_c}{\lambda}, \quad u_c = \frac{(1+\nu)h \alpha T_c}{1-\nu} \frac{1}{2}, \quad \sigma_c = \frac{E}{(1+\nu)(1-2\nu)} \frac{u_c}{h}, \quad \varepsilon_c = \frac{u_c}{h}, \quad (3.3)$$

and  $q_c$  denotes an amplitude of a thermal perturbation. The latter quantity is a base scale for the remaining field functions.<sup>3</sup> All the scales may be chosen arbitrarily; the presented scales were chosen in order to simplify the presentation and numerical treatment of the relationships for the considered fields.

Thus, the governing equations [Eq. (2.1)] in dimensionless general form read

$$\begin{aligned} \frac{\partial \bar{T}}{\partial \bar{t}} &= \bar{\nabla}^2 \bar{T} + \bar{q}, \\ (1-2\nu)\bar{\nabla}^2 \bar{u} + \bar{\nabla}(\bar{\nabla} \cdot \bar{u}) &= 4(1-\nu)\bar{\nabla} \bar{T}, \\ \bar{\sigma} &= (1-2\nu)\bar{\varepsilon} + \nu \text{Tr}(\bar{\varepsilon}) - 2(1-\nu)I\bar{T}, \\ \bar{\varepsilon} &= \frac{1}{2}[\bar{\nabla} \bar{u} + (\bar{\nabla} \bar{u})^T], \quad \text{Tr}(\bar{\varepsilon}) = \bar{\nabla} \cdot \bar{u}. \end{aligned} \quad (3.4)$$

These equations will be specified in detail according to the adopted assumptions in the suitable next Sections, namely the first one in Sect. 4. [Eq. (4.1)], the second one in Sect. 5. [Eq. (5.1)], and the remaining ones in Sect. 6. [the equations at the beginning of the Section].

Note that in the dimensionless equations there occurs only one material parameter, namely Poisson's coefficient  $\nu$ . If therefore no other parameters are introduced in the (dimensionless) boundary conditions [see later Sect. 4., Eqs. (4.2) and (4.3), and Sect. 5., Eq. (5.4)], then the considered fields are influenced only by Poisson's coefficient and by parameter (-s) of heat perturbation (in dimensionless description); all the remaining parameters of a problem are included in dimension scale factors. A dimensional quantity is therefore given by the product of the dimensionless quantity and its scale factor. In particular, the dependence of a given field on the layer thickness  $h$  is included in the proper scale factor (and also in the scale factors for time and spatial

<sup>3</sup> The scale  $q_c$  may be determined using the following relationships between  $q = q_c \bar{q}$  and total energy of perturbation  $Q$  (in case of perturbation of finite duration) or total perturbation rate  $\dot{Q}$  (in case of continuous perturbation):

$$Q = 2\pi t_c h^3 q_c \int_0^\infty \int_0^\infty \int_0^1 \bar{q} d\bar{r} d\bar{z}, \quad \dot{Q} = 2\pi h^3 q_c \int_0^\infty \int_0^1 \bar{q} \bar{r} d\bar{r} d\bar{z}$$

(if the type of perturbation is specified).

coordinates). For example, the scale factor of stress, as it follows from Eqs. (3.1), (3.3) and footnote 3, is proportional to

$$\sigma_c \propto \frac{E\alpha Q}{\rho ch^3} \quad \text{or} \quad \sigma_c \propto \frac{E\alpha \dot{Q}}{\lambda h}, \quad (3.5)$$

where the first relation holds in case of heat perturbation of finite duration ( $Q$  stands for the total energy of perturbation), and the second one in case of a continuous perturbation ( $\dot{Q}$  stands for the total perturbation rate).

In the further course, only dimensionless description will be applied, and a bar over the all variables will be omitted in the next Sections for simplicity.

#### 4 The thermal problem

According to the general assumptions adopted earlier, the heat conduction equation reads

$$\frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial z^2} + q. \quad (4.1)$$

The initial condition is assumed in the form:

$$T(t = 0) = 0. \quad (4.2)$$

The boundary conditions are assumed in two alternative versions (see Sect. 2):

- (a) both surfaces are insulated adiabatically, or
- (b) the external surface of the coating material is adiabatically insulated, and the internal surface is kept at temperature equal to zero:

$$\frac{\partial T}{\partial r}(r = 0) = 0 = T(r \rightarrow \infty) \quad (4.3)$$

and

$$\frac{\partial T}{\partial z}(z = 0) = 0 = \frac{\partial T}{\partial z}(z = 1), \quad (4.4.1)$$

or

$$\frac{\partial T}{\partial z}(z = 0) = 0 = T(z = 1). \quad (4.4.2)$$

The temperature field in the layer depends on the distribution of the heat perturbation term  $q$ . In case of a spatially limited perturbation, the temperature generally decreases with the distance from the perturbation region. The evolution of the temperature field depends on the time program of the heat perturbation.

The problem expressed by Eqs. (4.1)–(4.4) may be solved in a few ways. For our purposes, it is convenient to use suitable integral transformations with respect to spatial coordinates, namely the Hankel transformation of 0-th order with respect to variable  $r$ :

$$\psi^P := \int_0^\infty \psi(r) J_0(rp) r dr \quad (4.5)$$

( $J_0$  stands for the Bessel function of 0-th order), and the Fourier-cosine transformation with respect to variable  $z$ :

$$\psi^k := \int_0^1 \psi(z) \cos(\mu_k z) dz \quad (4.6)$$

where<sup>4</sup>

$$\mu_k := \begin{cases} k\pi & \text{—in case } a \\ (k + \frac{1}{2})\pi & \text{—in case } b. \end{cases} \quad (4.7)$$

After these transformations Eqs. (4.1)–(4.2) read

$$\frac{dT^{pk}}{dT} = -(p^2 + \mu_k^2)T^{pk} + q^{pk}, \quad T^{pk}(t=0) = 0.$$

The solution is

$$T^{pk} = \exp[-(p^2 + \mu_k^2)t] \int_0^t q^{pk}(t') \exp[(p^2 + \mu_k^2)t'] dt'. \quad (4.8)$$

Performing the inverse Hankel and Fourier transformations one may write the solution to the problem (4.1)–(4.4) in the form:

$$T^{(a)} = \int_0^\infty T^{p0} J_0(pr) p dp + 2 \sum_{k=1}^\infty \int_0^\infty T^{pk} J_0(pr) p dp \cos(k\pi z), \quad (4.9.1)$$

$$T^{(b)} = 2 \sum_{k=0}^\infty \int_0^\infty T^{pk} J_0(pr) p dp \cos\left[\left(k + \frac{1}{2}\right)\pi z\right] \quad (4.9.2)$$

in cases *a* and *b*, respectively.<sup>5</sup>

## 5 The displacement problem

According to the adopted assumptions, the displacement components  $u_r$  and  $u_z$  satisfy the following Lamé thermoelasticity equations ( $u_\varphi = 0$  by the symmetry) [16]:

$$\begin{aligned} \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u_r}{\partial r} \right) - \frac{u_r}{r^2} + \frac{\partial^2 u_r}{\partial z^2} + \frac{1}{1-2\nu} \frac{\partial}{\partial r} \nabla \cdot u &= \frac{4(1-\nu)}{1-2\nu} \frac{\partial T}{\partial r}, \\ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u_z}{\partial r} \right) + \frac{\partial^2 u_z}{\partial z^2} + \frac{1}{1-2\nu} \frac{\partial}{\partial z} \nabla \cdot u &= \frac{4(1-\nu)}{1-2\nu} \frac{\partial T}{\partial z}, \end{aligned} \quad (5.1)$$

where

$$\nabla \cdot u = \frac{1}{r} \frac{\partial(ru_r)}{\partial r} + \frac{\partial u_z}{\partial z} \quad (5.2)$$

and  $T$  is the solution of the heat conduction problem [Eqs. (4.1)–(4.4)] as given by Eq. (4.9).

The boundary conditions for the displacements  $u_r$  and  $u_z$  are assumed as follows:

- the external surface of the coating layer is stress free:  $\sigma_{rz}(z=0) = 0 = \sigma_{zz}(z=0)$ ,
- the substrate of the coating layer is rigid:  $u_r(z=1) = 0 = u_z(z=1)$ ,

<sup>4</sup> The proof of the orthogonality and of the completeness of the set  $\{\cos[(k + \frac{1}{2})\pi z], k = 0, 1, 2, \dots, z \in [0, 1]\}$  is given in Appendix A.

<sup>5</sup> The solution of the thermal problem in the form presented earlier is especially convenient to analyse processes in a range of long time. A solution obtained using the Green's function method (see Appendix B) may be more convenient for an analysis in a range of short time.

which after using the Duhamel–Neumann equation [Eqs. (2.1.3, 4)] yield

$$\begin{aligned} \frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r} &= 0, \quad \text{for } z = 0, \\ \nu \frac{1}{r} \frac{\partial(r u_r)}{\partial r} + (1 - \nu) \frac{\partial u_z}{\partial z} - 2(1 - \nu)T &= 0, \quad \text{for } z = 0, \\ u_r &= 0, \quad \text{for } z = 1, \\ u_z &= 0, \quad \text{for } z = 1, \end{aligned} \quad (5.3)$$

– and the displacement field vanishes at infinity ( $u_r = 0 = u_z$  for  $r \rightarrow \infty$ ).

The following procedure is applied to solve this problem.<sup>6</sup> Applying the Hankel transformation of the 1st order with respect to variable  $r$  to Eqs. (5.1.1), (5.3.1), and (5.3.3) and that transformation of 0-th order (with respect to variable  $r$ ) to Eqs. (5.1.2), (5.3.2), and (5.3.4) one may rewrite the problem expressed by Eqs. (5.1)–(5.3) in the form:

$$-2(1 - \nu)p^2 \tilde{u}_r^p + (1 - 2\nu) \frac{\partial^2 \tilde{u}_r^p}{\partial z^2} - p \frac{\partial u_z^p}{\partial z} = -4(1 - \nu)pT^p, \quad (5.4.1)$$

$$p \frac{\partial \tilde{u}_r^p}{\partial z} - (1 - 2\nu)p^2 u_z^p + 2(1 - \nu) \frac{\partial^2 u_z^p}{\partial z^2} = 4(1 - \nu) \frac{\partial T^p}{\partial z} \quad (5.4.2)$$

and

$$\begin{aligned} \frac{\partial \tilde{u}_r^p}{\partial z} - p u_z^p &= 0, \quad \text{for } z = 0, \\ \nu p \tilde{u}_r^p + (1 - \nu) \frac{\partial u_z^p}{\partial z} &= 2(1 - \nu)T^p, \quad \text{for } z = 0, \\ \tilde{u}_r^p &= 0, \quad \text{for } z = 1, \\ u_z^p &= 0, \quad \text{for } z = 1, \end{aligned} \quad (5.5)$$

where the Hankel transforms  $T^p$  and  $u_z^p$  of the functions  $T$  and  $u_z$  are defined by Eq. (4.5), and that transform of the function  $u_r$  is defined as

$$\tilde{u}_r^p := \int_0^\infty u_r J_1(rp) r dr, \quad (5.6)$$

where, in turn,  $J_1$  stands for the Bessel function of the 1-st order; note that according to Eq. (4.9) the Hankel transform of the function  $T$  is given by the formulae:

$$T^{p(a)} = T^{p0} + 2 \sum_{k=1}^\infty T^{pk} \cos(k\pi z), \quad (5.7.1)$$

$$T^{p(b)} = 2 \sum_{k=0}^\infty T^{pk} \cos[(k + \frac{1}{2})\pi z], \quad (5.7.2)$$

in cases  $a$  and  $b$ , respectively, where  $T^{pk}$  are given by Eq. (4.8).

Equation (5.4) represents the set of ordinary differential equations (time occurs here as a parameter). Their general solution may be written in the form:<sup>7</sup>

$$\begin{aligned} \tilde{u}_r^p &= \left[ A \left( z - \frac{3 - 4\nu}{2p} \right) + C \right] e^{-pz} + \left[ B \left( z + \frac{3 - 4\nu}{2p} \right) + D \right] e^{pz} + F1 - F2, \\ u_z^p &= \left[ A \left( z + \frac{3 - 4\nu}{2p} \right) + C \right] e^{-pz} - \left[ B \left( z - \frac{3 - 4\nu}{2p} \right) + D \right] e^{pz} + F1 + F2, \end{aligned} \quad (5.8)$$

<sup>6</sup> Rudin [13] solved some particular problems of this type by a special assumption on the structure of sought solution. We apply a more general procedure, which does not require such an assumption, and leads to the results in a simpler form. In the case considered by Rudin, the final results in both approaches are equivalent.

<sup>7</sup> For some details see Appendix C.

where  $A, B, C, D$  are integration constants, and

$$\begin{aligned}
 F1 &:= e^{-pz} \int_0^z e^{pz'} T^p(z') dz' \\
 &= \begin{cases} T^{p0} \frac{1 - e^{-pz}}{p} + 2 \sum_{k=1}^{\infty} \frac{pT^{pk}}{p^2 + \mu_k^2} [\cos(\mu_k z) + \frac{\mu_k}{p} \sin(\mu_k z) - e^{-pz}], & \text{-- case a} \\ 2 \sum_{k=0}^{\infty} \frac{pT^{pk}}{p^2 + \mu_k^2} [\cos(\mu_k z) + \frac{\mu_k}{p} \sin(\mu_k z) - e^{-pz}], & \text{-- case b} \end{cases} \\
 F2 &:= e^{pz} \int_0^z e^{-pz'} T^p(z') dz' \\
 &= \begin{cases} -T^{p0} \frac{1 - e^{pz}}{p} - 2 \sum_{k=1}^{\infty} \frac{pT^{pk}}{p^2 + \mu_k^2} [\cos(\mu_k z) - \frac{\mu_k}{p} \sin(\mu_k z) - e^{pz}], & \text{-- case a} \\ 2 \sum_{k=0}^{\infty} T^{pk} \frac{pT^{pk}}{p^2 + \mu_k^2} [-\cos(\mu_k z) + \frac{\mu_k}{p} \sin(\mu_k z) + e^{pz}], & \text{-- case b} \end{cases}
 \end{aligned} \tag{5.9}$$

where, in turn,  $\mu_k$  is given by Eq. (4.7).

The integration constants  $A, B, C, D$  are determined from the boundary conditions. Substituting Eq. (5.8) into Eq. (5.5), one obtains the following set of algebraic equations for these constants:

$$\begin{aligned}
 & \begin{matrix} A & & +B & & -2pC & +2pD = 0, \\ & -A & & +B & -2pC & -2pD = 0, \end{matrix} \\
 A \left( 1 - \frac{3-4\nu}{2p} \right) e^{-p} & + B \left( 1 + \frac{3-4\nu}{2p} \right) e^p + C e^{-p} + D e^p = R1, \\
 A \left( 1 + \frac{3-4\nu}{2p} \right) e^{-p} & - B \left( 1 - \frac{3-4\nu}{2p} \right) e^p + C e^{-p} - D e^p = R2,
 \end{aligned} \tag{5.10}$$

where

$$\begin{aligned}
 R1 &:= -(F1 - F2)(z = 1) \\
 &= \begin{cases} T^{p0} \frac{-2 + e^{-p} + e^p}{p} + 2 \sum_{k=1}^{\infty} \frac{pT^{pk}}{p^2 + \mu_k^2} [-2(-1)^k + e^{-p} + e^p], & \text{-- case a} \\ -2 \sum_{k=0}^{\infty} \frac{pT^{pk}}{p^2 + \mu_k^2} (e^{-p} + e^p), & \text{-- case b} \end{cases} \\
 R2 &:= -(F1 + F2)(z = 1) \\
 &= \begin{cases} T^{p0} \frac{e^{-p} - e^p}{p} + 2 \sum_{k=1}^{\infty} \frac{pT^{pk}}{p^2 + \mu_k^2} (e^{-p} - e^p), & \text{-- case a} \\ 2 \sum_{k=0}^{\infty} \frac{pT^{pk}}{p^2 + \mu_k^2} [-2(-1)^k \frac{\mu_k}{p} + e^{-p} - e^p], & \text{-- case b} \end{cases}
 \end{aligned} \tag{5.11}$$

where, in turn,  $\mu_k$  is given by Eq. (4.7). The solution of this set of algebraic equations is

$$\begin{aligned}
 A &= p \frac{-R1\{e^{-p} - [2p - (3 - 4\nu)]e^p\} + R2\{e^{-p} + [2p + (3 - 4\nu)]e^p\}}{1 + (3 - 4\nu)^2 + 4p^2 + (3 - 4\nu)(e^{-2p} + e^{2p})}, \\
 B &= p \frac{R1\{[2p + (3 - 4\nu)]e^{-p} + e^p\} - R2\{[2p - (3 - 4\nu)]e^{-p} - e^p\}}{1 + (3 - 4\nu)^2 + 4p^2 + (3 - 4\nu)(e^{-2p} + e^{2p})}, \\
 C &= \frac{1}{2p} B, \quad D = -\frac{1}{2p} A,
 \end{aligned} \tag{5.12}$$

where  $R1, R2$  are given by Eq. (5.11).

Substituting these integration constants into Eq. (5.8) and next performing the suitable inverse Hankel transformations, one obtains the displacement vector components in the form:

$$u_r = \int_0^{\infty} \tilde{u}_r^p J_1(rp) p dp, \quad u_z = \int_0^{\infty} u_z^p J_0(rp) p dp, \quad (5.13)$$

where  $\tilde{u}_r^p$  and  $u_z^p$  are given by Eq. (5.8) with Eq. (5.12) and with Eqs. (5.7) and (4.8).

## 6 The stress field

The components of strain are given by the formulae [17] (in our case  $u_\varphi = 0 = \varepsilon_{r\varphi} = \varepsilon_{\varphi z}$  by the symmetry):

$$\varepsilon_{rr} = \frac{\partial u_r}{\partial r}, \quad \varepsilon_{rz} = \frac{1}{2} \left( \frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r} \right), \quad \varepsilon_{\varphi\varphi} = \frac{1}{r} u_r, \quad \varepsilon_{zz} = \frac{\partial u_z}{\partial z}, \quad (6.1)$$

and the trace of strain is

$$Tr\varepsilon = \nabla \cdot u = \frac{1}{r} \frac{\partial r u_r}{\partial r} + \frac{\partial u_z}{\partial z}. \quad (6.2)$$

The stress components are given by the formulae according to Eq. (3.4.3):

$$\begin{aligned} \sigma_{rr} &= (1 - 2\nu)\varepsilon_{rr} + \nu \nabla \cdot u - 2(1 - \nu)T, & \sigma_{r\varphi} &= 0, & \sigma_{rz} &= (1 - 2\nu)\varepsilon_{rz}, \\ \sigma_{\varphi\varphi} &= (1 - 2\nu)\varepsilon_{\varphi\varphi} + \nu \nabla \cdot u - 2(1 - \nu)T, & \sigma_{\varphi z} &= 0, \\ \sigma_{zz} &= (1 - 2\nu)\varepsilon_{zz} + \nu \nabla \cdot u - 2(1 - \nu)T. \end{aligned} \quad (6.3)$$

Using these relationships and Eq. (5.13), we have therefore for the stress components

$$\begin{aligned} \sigma_{rr} &= \int_0^{\infty} \left\{ \left[ (1 - \nu) p \tilde{u}_r^p + \nu \frac{\partial u_z^p}{\partial z} - 2(1 - \nu) T^p \right] J_0(rp) - (1 - 2\nu) \frac{1}{r} \tilde{u}_r^p J_1(rp) \right\} p dp, \\ \sigma_{rz} &= \frac{1 - 2\nu}{2} \int_0^{\infty} \left( \frac{\partial \tilde{u}_r^p}{\partial z} - p u_z^p \right) J_1(rp) p dp, \\ \sigma_{\varphi\varphi} &= \int_0^{\infty} \left\{ \left[ \nu p \tilde{u}_r^p + \nu \frac{\partial u_z^p}{\partial z} - 2(1 - \nu) T^p \right] J_0(rp) + (1 - 2\nu) \frac{1}{r} \tilde{u}_r^p J_1(rp) \right\} p dp, \\ \sigma_{zz} &= \int_0^{\infty} \left[ \nu p \tilde{u}_r^p + (1 - \nu) \frac{\partial u_z^p}{\partial z} - 2(1 - \nu) T^p \right] J_0(rp) p dp, \end{aligned} \quad (6.4)$$

where the function  $T^p$  is given by Eq. (5.7) with Eq. (4.8); the functions  $\tilde{u}_r^p$  and  $u_z^p$  are given by Eq. (5.8) with Eq. (5.9) [with Eq. (4.8)] and Eq. (5.12) [with Eq. (5.11) [with Eq. (4.8)]]; properties (derivatives) of Bessel functions were used; and derivatives of the functions  $\tilde{u}_r^p$  and  $u_z^p$  are given by the following formulae:

$$\frac{\partial \tilde{u}_r^p}{\partial z} = A \left[ \left( \frac{5}{2} - 2\nu - pz \right) e^{-pz} - \frac{1}{2} e^{pz} \right] + B \left[ -\frac{1}{2} e^{-pz} + \left( \frac{5}{2} - 2\nu + pz \right) e^{pz} \right] - p(F1 + F2), \quad (6.5)$$

$$\frac{\partial u_z^p}{\partial z} = A \left[ \left( -\frac{1}{2} + 2\nu - pz \right) e^{-pz} + \frac{1}{2} e^{pz} \right] - B \left[ \frac{1}{2} e^{pz} + \left( -\frac{1}{2} + 2\nu + pz \right) e^{-pz} \right] - p(F1 - F2) + 2T^p$$

(with suitable formulae determining the constants  $A, B$  and the functions  $F1, F2$ —identical with those for the functions  $\tilde{u}_r^p, u_z^p$  mentioned above).



Thus, we obtained general formulae which allow us to analyze the evolution of the stress tensor in a coating layer as modeled in Sect. 2, if the thermal perturbation is specified (and if also the coating material is specified; however, in dimensionless description the only material parameter which has to be taken into account is the Poisson's coefficient  $\nu$ , so specification of the material is very simple and is realizable in a relatively narrow range). In each case of specific perturbation, the analysis of the evolution of stress requires some numerical work. Such an analysis for perturbations modeling realistic situations will be presented in Part II of the paper. At the end of Part I, only a simple example is given as an illustration of effectiveness of the presented theoretical scheme.

## 7 Simple illustrative example

Let the heat perturbation be an instantaneous surface point pulse:

$$q = \delta(t) \frac{\delta(r)}{r} \delta(z) \quad (7.1)$$

[ $\delta(x)$  stands for the Dirac delta distribution]. The Poisson coefficient is assumed to be equal to  $\nu = 0.3$  as a representative value. The aim is to calculate the evolution of the tangent and normal components of the stress tensor  $\sigma_{rz}$  and  $\sigma_{zz}$  in the layer at its contact surface with the substrate, i.e. for  $z = 1$ , in case *a*; the evolution of the distribution of the temperature is calculated and presented first for orientation.

The accuracy of the numerical calculations and that of truncation of the series in each suitable time region were chosen in such a way as to assure that errors in the final results do not exceed  $5 \cdot 10^{-4}$  (four significant digits).

In the considered case, the Hankel–Fourier transform of heat perturbation is equal to  $q^{pk} = \delta(t)$ , and that the transform of temperature [see Eq. (4.8)] is equal to

$$T^{pk} = \exp[-(p^2 + k^2\pi^2)t], \quad (7.2)$$

therefore from Eq. (4.9.1) we have

$$T^{(a)}(z = 1) = \frac{1}{2t} \exp\left[-\frac{r^2}{4t}\right] \left\{ 1 + 2 \sum_{k=1}^{\infty} (-1)^k \exp[-k^2\pi^2 t] \right\}, \quad (7.3)$$

where the formula

$$\int_0^{\infty} \exp[-p^2 t] J_0(rp) p dp = \frac{1}{2t} \exp\left[-\frac{r^2}{4t}\right] \quad (7.4)$$

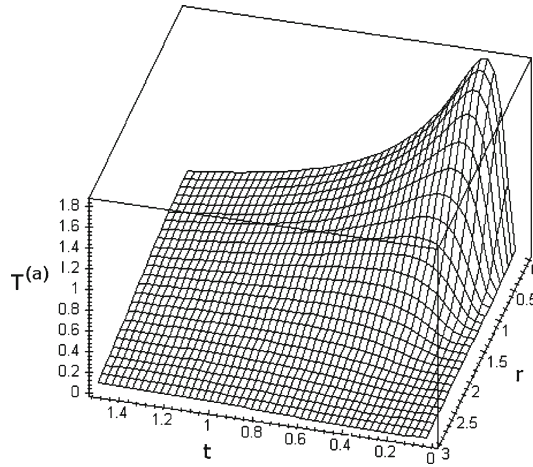
was used [18]. This formula was used in calculations in the long and middle time regions; in the short time region Eq. (B.1) (see Appendix B) was used. The behavior of the temperature distribution is presented in Fig. 1.

The stress tensor components [see Eq. (6.4)] in the considered case are given by the formulae:

$$\begin{aligned} \sigma_{rz}^{(a)}(z = 1) &= 0.2 \int_0^{\infty} \frac{\partial \tilde{u}_r^p}{\partial z}(z = 1) J_1(rp) p dp, \\ \sigma_{zz}^{(a)}(z = 1) &= 0.7 \int_0^{\infty} \left[ \frac{\partial u_z^p}{\partial z} - 2T^p \right](z = 1) J_0(rp) p dp \end{aligned} \quad (7.5)$$

[where Eqs. (5.5.3, 4) were used] with [see Eq. (6.5)]

$$\begin{aligned} \frac{\partial \tilde{u}_r^p}{\partial z}(z = 1) &= A \left[ (1.9 - p)e^{-p} - \frac{1}{2}e^p \right] + B \left[ -\frac{1}{2}e^{-p} + (1.9 + p)e^p \right] + pR2, \\ \left[ \frac{\partial u_z^p}{\partial z} - 2T^p \right](z = 1) &= A \left[ (0.1 - p)e^{-p} + \frac{1}{2}e^p \right] - B \left[ \frac{1}{2}e^{-p} + (0.1 + p)e^p \right] + pR1, \end{aligned} \quad (7.6)$$



**Fig. 1** Evolution of distribution of  $T^{(a)}(t, r)$  (at the surface  $z = 1$ )

where the constants  $A, B$  are given by Eq. (5.12) with Eq. (5.11) in parts concerning case  $a$  with  $T^{pk}$  specified by Eq. (7.2).

Analogous formulae for stresses may be obtained starting with the temperature given by Eq. (B.1). The procedure is the same with only  $R1$  and  $R2$  given by the following formulae instead of Eq. (5.11) (in detailed form in parts concerning case  $a$ ):

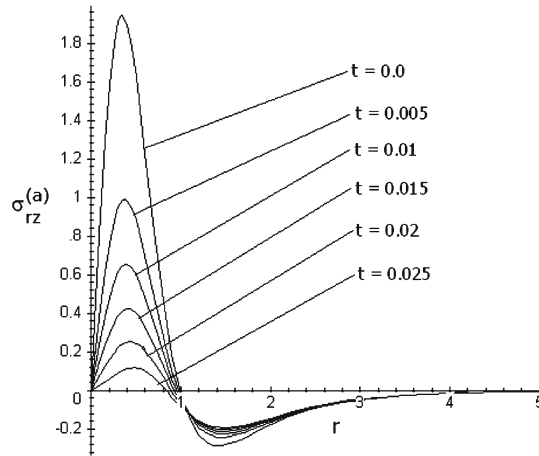
$$\begin{aligned}
 R1 &= \sum_{m=0}^{\infty} \left\{ e^{-(2m+1)p} \left[ 2\operatorname{erf} \left( p\sqrt{t} - \frac{2m+1}{2\sqrt{t}} \right) - \operatorname{erf} \left( p\sqrt{t} - \frac{m+1}{\sqrt{t}} \right) - \operatorname{erf} \left( p\sqrt{t} - \frac{m}{\sqrt{t}} \right) \right] \right. \\
 &\quad \left. + e^{(2m+1)p} \left[ 2\operatorname{erf} \left( p\sqrt{t} + \frac{2m+1}{2\sqrt{t}} \right) - \operatorname{erf} \left( p\sqrt{t} + \frac{m+1}{\sqrt{t}} \right) - \operatorname{erf} \left( p\sqrt{t} + \frac{m}{\sqrt{t}} \right) \right] \right\}, \\
 R2 &= \sum_{m=0}^{\infty} \left\{ e^{-(2m+1)p} \left[ \operatorname{erf} \left( p\sqrt{t} - \frac{m+1}{\sqrt{t}} \right) - \operatorname{erf} \left( p\sqrt{t} - \frac{m}{\sqrt{t}} \right) \right] \right. \\
 &\quad \left. + e^{(2m+1)p} \left[ -\operatorname{erf} \left( p\sqrt{t} + \frac{m+1}{\sqrt{t}} \right) + \operatorname{erf} \left( p\sqrt{t} + \frac{m}{\sqrt{t}} \right) \right] \right\}.
 \end{aligned} \tag{7.7}$$

The calculated evolution of the stress component  $\sigma_{rz}^{(a)}$  is presented in Figs. 2, 3, 4. It evolves in two stages: (i) it relatively quickly decreases from maximum  $\sigma_{rz}^{(a)}(\max) = 1.943$  (at  $r = 0.3417, t = 0$ ) to minimum  $\sigma_{rz}^{(a)}(\min) = -0.4688$  (for  $r = 0.5286, t = 0.1024$ ), and (ii) next it relatively slowly relaxes to 0. Because of different changes and rates of  $\sigma_{rz}^{(a)}$ , it is convenient to present its evolution in three Figures using different scales in each time regime.

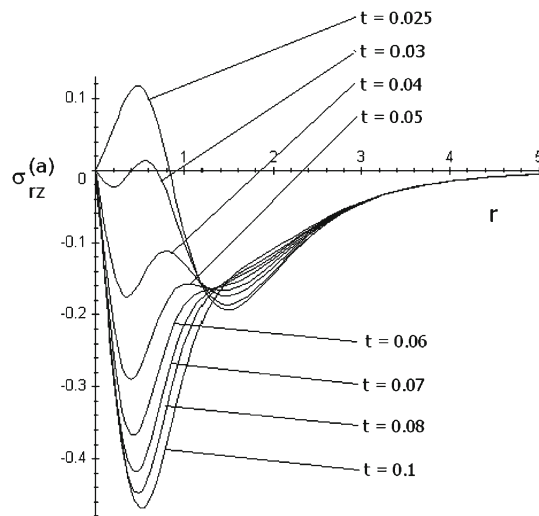
Such a behavior of  $\sigma_{rz}^{(a)}$  may be interpreted as an effect of competition of two mechanisms: (i) a trend to tuck up the lower parts of the layer due to heterogeneous thermal expansion generated by heterogeneous distribution of temperature, which causes a tension action of the substrate, and (ii) the usual thermal expansion due to an increase of temperature, which causes a pull action of the substrate. Initially, when the distribution of the temperature is strongly heterogeneous, the first mechanism dominates. Next, when the temperature distribution becomes less heterogeneous with time, the first mechanism becomes weaker and weaker, and the second mechanism begins to dominate.

The evolution of  $\sigma_{zz}^{(a)}$  is more complicated. Because of different changes and rates of  $\sigma_{zz}^{(a)}$  it is convenient to present its evolution in four Figures (Figs. 5, 6, 7, 8) using different scales in each time regime.  $\sigma_{zz}^{(a)}$  relaxes with time from the initial distribution (for  $t = 0$ ) with relatively large maximum  $\sigma_{zz}^{(a)}(\max) = 7.852$  (at  $r = 0$ ) and minimum  $\sigma_{zz}^{(a)}(\min) = -0.4819$  (at  $r = 1.115$ ), approaching in the meantime the additional lower maximum and additional shallower minimum.

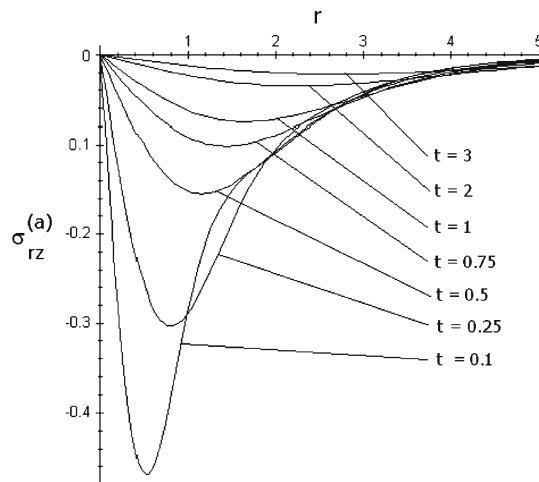
Such a behavior of  $\sigma_{zz}^{(a)}$  may be interpreted as an effect of competition of two mechanisms: (i) a trend to keep a locally expanding element of the layer on a substrate by surrounding elements due to heterogeneous



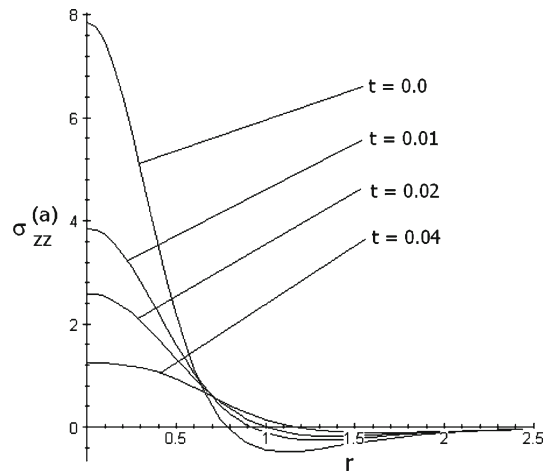
**Fig. 2** Evolution of  $\sigma_{rz}^{(a)}(t, r, z = 1)$  at the beginning (for very short time  $0 \leq t \leq 0.025$ )



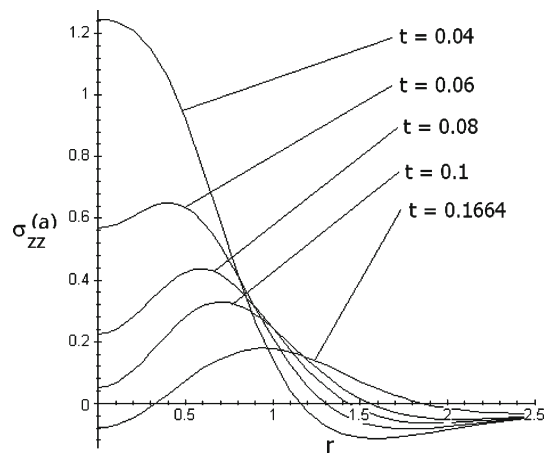
**Fig. 3** Evolution of  $\sigma_{rz}^{(a)}(t, r, z = 1)$  after the beginning and before approaching the minimum (for middle time  $0.025 \leq t \leq 0.1$ )



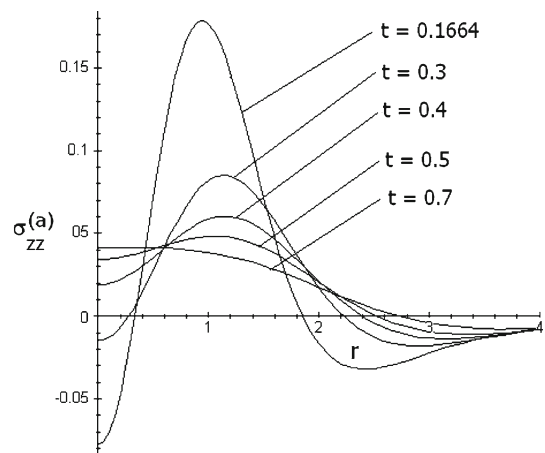
**Fig. 4** Relaxation of  $\sigma_{rz}^{(a)}(t, r, z = 1)$  from minimum to 0 ( $t \geq 0.1$ )



**Fig. 5** Evolution of  $\sigma_{zz}^{(a)}(t, r, z = 1)$  in the period  $0 \leq t \leq 0.04$

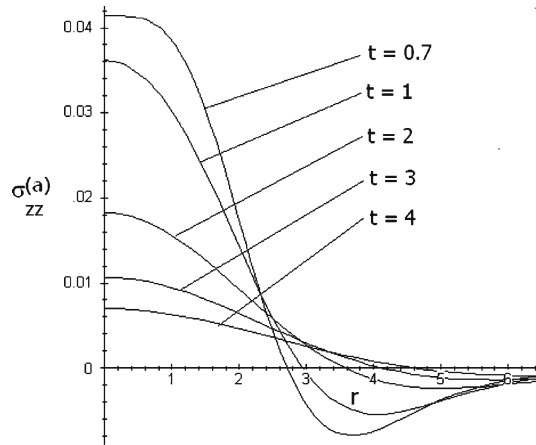


**Fig. 6** Evolution of  $\sigma_{zz}^{(a)}(t, r, z = 1)$  in the period  $0.04 \leq t \leq 0.1664$



**Fig. 7** Evolution of  $\sigma_{zz}^{(a)}(t, r, z = 1)$  in the period  $0.1664 \leq t \leq 0.7$

thermal expansion generated by a heterogeneous distribution of temperature, which causes a local thrust of the layer on the substrate, and (ii) a non-uniform thermal expansion due to a non-uniform increase of temperature, which causes a delamination trend in the system. Competition of these mechanisms produces varying maxima and minima of  $\sigma_{zz}^{(a)}$ .



**Fig. 8** Evolution of  $\sigma_{zz}^{(a)}(t, r, z = 1)$  for  $t \geq 0.7$

Of course, for sufficiently long time the temperature approaches the initial homogeneous distribution, and the layer approaches a stress free state.

At the end of this Section let us note that some spectacular features of behavior of stresses may be caused by the special type of heat perturbation (in this case the initial temperature at the center on the free surface is infinite!), and assumed rigidity of the substrate. The first aspect will be explained in Part II of the paper where more realistic perturbations will be examined.

**Appendix A: The orthogonality and completeness of the set**

$$\left\{ \psi_k = \sqrt{2} \cos \left[ \left( k + \frac{1}{2} \right) \pi z \right], k = 0, 1, 2, \dots, z \in [0, 1] \right\}$$

The orthogonality of the set may be verified in a simple way. In fact, after some algebra one may obtain for the scalar product  $(\psi_k, \psi_m)$

$$(\psi_k, \psi_m) = \int_0^1 \psi_k \psi_m dz = 2 \int_0^1 \cos \left[ \left( k + \frac{1}{2} \right) \pi z \right] \cos \left[ \left( m + \frac{1}{2} \right) \pi z \right] dz = \delta_{km}, \tag{A.1}$$

where  $\delta_{km}$  stands for the Kronecker delta.

The completeness of this set may be proved by verification of the Parseval equality (see [19]). Since the set  $\{\varphi_k = \sqrt{2} \sin(k\pi z), k = 1, 2, 3, \dots, z \in [0, 1]\}$  is a complete orthogonal set (see [19]), it is sufficient to verify the Parseval equality for functions  $\varphi_k$  as expressed in the base  $\{\psi_k\}$ . Thus, in order to prove the completeness of the set under consideration we have to verify that the Parseval equality

$$(\varphi_k, \varphi_k) = \sum_{m=0}^{\infty} (\varphi_k, \psi_m)^2 \tag{A.2}$$

takes place. In the considered case this equality reads

$$2 \int_0^1 \sin^2(k\pi z) dz = 4 \sum_{m=0}^{\infty} \left[ \int_0^1 \sin(k\pi z) \cos \left[ \left( m + \frac{1}{2} \right) \pi z \right] dz \right]^2. \tag{A.3}$$

By performing integration one may prove that the left-hand side of the latter formula is equal to unity, and the right-hand side to

$$\frac{16(2k)^2}{\pi^2} \sum_{m=0}^{\infty} [(2m + 1)^2 - (2k)^2]^{-2}. \tag{A.4}$$

Because the series is equal to reciprocity of the factor before it (see [20]), the Parseval equality is satisfied for the examined set, which proves that this set is a complete one.

### Appendix B: Green's function for the thermal problem in a layer

The Green's function for the thermal problem in a half space is twice such a function in case of a full space, which is known (see for example [21]). Applying the method of sources and sinks (also known as the method of images) [21] one may obtain the Green's function for the thermal problem in a flat infinite layer [22] [for heat source  $q = \delta(t) \frac{1}{r} \delta(r) \delta(z)$ ]

$$T_G = \frac{1}{2\sqrt{\pi}} \frac{1}{\sqrt{t^3}} \exp\left[-\frac{r^2}{4t}\right] \sum_{m=0}^{\infty} (-1)^{sm} \left\{ \exp\left[-\frac{(2m+z)^2}{4t}\right] + (-1)^s \exp\left[-\frac{[2(m+1)-z]^2}{4t}\right] \right\}, \quad (\text{B.1})$$

where  $s = 0$  in case *a* and  $s = 1$  in case *b*. For another heat source the solution is given by convolution of Green's function and the heat source:  $T = T_G * q$ .

### Appendix C: Some details concerning the solution as expressed by Eq. (5.8)

After operation  $\frac{\partial}{\partial z}(5.4.1) + p(5.4.2)$  we have  $(\tilde{u}_{r,z}^p + pu_z^p)_{,zz} - p^2(\tilde{u}_{r,z}^p + pu_z^p) = 0$ , where  $f_{,z}$  stands for (partial) derivative of  $f$  with respect to  $z$ , from which

$$\tilde{u}_{r,z}^p + pu_z^p = ae^{-pz} + be^{pz}, \quad (\text{C.1})$$

where  $a$  and  $b$  stand for integration constants.

Adding and subtracting the term  $(1 - 2\nu)pu_{z,z}^p$  to the left-hand side of Eq. (5.4.1) and using Eq. (C.1) one may obtain

$$p\tilde{u}_r^p + u_{z,z}^p = \frac{1 - 2\nu}{2(1 - \nu)} (-ae^{-pz} + be^{pz}) + 2T^p. \quad (\text{C.2})$$

Adding and subtracting Eqs. (C.1) and (C.2) one obtains two independent ordinary differential equations of the 1st order for  $\tilde{u}_r^p \pm u_z^p$ . Solving these equations and next adding and subtracting the solutions one obtains finally the results as expressed by Eq. (5.8).

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