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BALANCE BOUNDARY CONDITIONS FOR THIN BOUNDARY LAYERS: DERIVATION FROM THE INTEGRAL CONJUGATION CONDITIONS

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Abstract: This study proposes a methodology for deriving boundary conditions in the presence of boundary layers by using integral conjugation conditions for thin geobarriers. These boundary conditions are essential part of the boundary value problems such as mathematical models of physical, chemical and hydrological processes. The developed approach allows to account for variable characteristics of the boundary layer material. Such consideration is significant in mathematical and computer modelling of environmental processes with strong nonlinear effects. By applying the proposed methodology, we derive balance boundary conditions for: soil surface moisture and temperature in case the soil is covered with growing crops or a layer of fallen leaves; salt concentration in pore water under carst processes; greenhouse gas distribution on the soil-atmosphere contact in the presence of growing plants.

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1. Introduction

Boundary conditions constitute an essential part of mathematical physics equa-

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tions, which are used for simulation and analysis of physical, chemical and hydrological processes in natural and artificial environments. The transitions from a real process to mathematical model and further to boundary value problem is accompanied by numerous assumptions concerning both the partial differential equations (PDEs) and their boundary conditions.

In this paper, we mostly discuss the problem in the view of interaction processes between heat fluxes in 'soil – atmosphere' environment. The corresponding model can be applied to simulating and forecasting the temperature of fertile soil layer, a problem relevant in agriculture [1, 2, 3, 4]. The obvious way to set the boundary condition for the soil-atmosphere interface is to use Newton-Richmann heat exchange law, or, even simpler, to assume that the soil surface temperature equals to the air temperature know from the meteorological measurements. However, in case there is a (presumably) thin layer of crops or snow that is defined by its own thermal capacity and conductivity characteristics, the application of these conditions requires additional justification. For example, if the modelling is carried out in real-time with meteorological air temperature data (which is typically measured 2m above the ground), we disregard the effect of crop cover and its warming due to the solar radiation [5, 6]. Similar doubts about the classical boundary conditions arise for the problem of tracking moisture of the fertile soil layer profile, when precipitation amounts or remotely sensed soil moisture data are available [7, 8, 9]. In this case, the amount of soil evaporation and transpiration depends also on the crop height and temperature. Thus, the task of producing realistic simulation and forecast in the real time calls for modification of boundary conditions to incorporate a notion of boundary layers, which have different characteristics from that of the problem medium.

2. Conjugation condition for the heat transfer with a thin layer on the soil-atmosthere contact

Here we propose methodology for deriving boundary conditions in the presence of thin boundary layers based on the integral conjugation conditions for geobarriers. Similar modifications for conjugation conditions with nonlinear dependencies are introduced in works [10, 11, 12, 13]. Further, studies [14, 15] adjust the conjugation conditions for thin inclusion to consider the effect of biocolmatation according to the methodology of modelling interconnected processes in porous media described in [16].

To preserve the logic and wholeness of the derivations, we summarize here

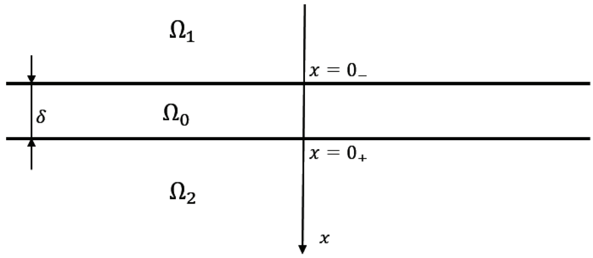

Figure 1: Thin geobarrier Ω_0 on the contact of two domains, Ω_1 and Ω_2

some of the known facts as for the temperature conjugation conditions provided in [10, 11, 12, 14, 15, 17]. In Figure 1, Ω_1 is atmosphere, Ω_2 – soil; Ω_0 – thin boundary layer with thickness δ, positioned at $x = 0$, where the heat transfer process is transpiring. Thermal and physical characteristics of materials in the domains Ω_0, Ω_1, Ω_2 differ from each other and can nonlinearly depend on the temperature itself. We assume, due to the thinness of the boundary layer, that thermal processes in the cross-section of the layer are stationary or, at least, quasi-stationary. Thus, we consider the following heat transfer problem for the layer:

$$\frac{\partial}{\partial x}\left(-\lambda_\delta\left(T\right)\frac{\partial T}{\partial x}\right) = 0, 0 < x < \delta, \tag{1}$$

$$T|_{x=0} = T^-, T|_{x=\delta} = T^+. \tag{2}$$

Here T is temperature, $\lambda_\delta\left(T\right)$ – thermal conductivity coefficient for the thin layer that can nonlinearly depend on temperature. Note that thermal conductivity can potentially depend, in addition, on other fields such as moisture, organic compounds, concentration of chemicals etc.

From equation (1) we get

$$\lambda_\delta\left(T\right)\frac{\partial T}{\partial x} = T_1,$$

where $T_1 = const$ is a yet unknown constant or a function of time t (the variance with time does not lead to significant differences in further derivation). Further,

$$T\left(x\right)=T_1\int_0^x\frac{dx}{\lambda_\delta\left(T\right)}+T_2, \tag{3}$$

where $T_2 = const$ is another yet unknown constant. Then, from (3) and boundary conditions (2) we have

$$\begin{cases} T\left(0\right)=T_2=T^-, \\ T\left(\delta\right)=T_1\int_0^\delta\frac{dx}{\lambda_\delta\left(T\right)}+T_2=T^+. \end{cases}$$

This system of linear algebraic equations leads to

$$T_2=T^-,\quad T_1=\frac{T^+-T^-}{\int_0^\delta\frac{dx}{\lambda_\delta(T)}}.$$

Thus, the problem (1), (2) yields

$$T\left(x\right)=\frac{T^+-T^-}{\int_0^\delta\frac{dx}{\lambda_\delta(T)}}\int_0^x\frac{dx}{\lambda_\delta\left(T\right)}+T^-.$$

Consequently, we get

$$\frac{\partial T}{\partial x}=\frac{T^+-T^-}{\lambda_\delta\left(T\right)\int_0^\delta\frac{dx}{\lambda_\delta(T)}}. \tag{4}$$

Then we derive conjugation condition from the conservation law for heat flux q:

$$q|_{x=0_\pm}=-\lambda_\delta\left(T\right)\frac{\partial T}{\partial x}. \tag{5}$$

Considering the Ox axis is directed downward, from (4) and (5) we have the final equation for modified conjugation condition on non-ideal contact for temperature on a thin boundary layer:

$$\lambda\left(T\right)\frac{\partial T}{\partial x}\bigg|_{x=0_\pm}=-\frac{T^+-T^-}{\int_0^\delta\frac{dx}{\lambda_\delta(T)}}. \tag{6}$$

Here $\lambda\left(T\right)$ is thermal conductivity of the material in domain Ω_1 (on $x=0_-$) or domain Ω_2 (on $x=0_+$). Condition (6) is part of the mathematical model for interconnected heat transfer processes in domains Ω_1 and Ω_2 with thin inclusion Ω_0. In case temperature field in one of the domains (Ω_1 for instance) is known, the thin inclusion Ω_0 becomes a boundary layer, and condition (6) becomes boundary condition after necessary modifications.

3. Balance boundary conditions

3.1. Heat transfer in the 'soil–atmosphere' environment in the presence of thin boundary layer (plants, snow, fallen leaves and pine needles etc.)

Temperature T^- is in this case known and equal to the air temperature T_a. Temperature T^+ is an unknown temperature T at the soil surface. Then, from the conjugation condition (6) we get the following boundary condition:

$$\lambda (T) \left. \frac{\partial T}{\partial x} \right|_{x=0} = - \frac{T|_{x=0} - T_a}{\int_0^\delta \frac{dx}{\lambda_\delta (T)}}, \tag{7}$$

where $\lambda_\delta (T)$ is thermal conductivity of the boundary layer material (plants, snow, plant litter). Assuming $\lambda_\delta (T) = \lambda_\delta = const$ yields

$$\lambda (T) \left. \frac{\partial T}{\partial x} \right|_{x=0} = -\lambda_\delta \frac{T|_{x=0} - T_a}{\delta}. \tag{8}$$

3.2. Moisture transfer in the 'soil–atmosphere' environment in the presence of thin boundary layer

In the study [17], according to Darcy-Klute law with gravitational flow [8], the following conjugation condition for moisture transfer equation can be derieved (where soil moisture is represented by pressure head h):

$$\left. \left(k(h) \frac{\partial h}{\partial x} - k(h) \right) \right|_{x=0_\pm} = - \frac{h^+ - h^-}{\int_0^\delta \frac{dx}{k_\delta (h)}} + \frac{\delta}{\int_0^\delta \frac{dx}{k_\delta (h)}}.$$

Then, as in (7), we get the following boundary condition:

$$\left. \left(k(h) \frac{\partial h}{\partial x} - k(h) \right) \right|_{x=0} = - \frac{h|_{x=0} - h_a}{\int_0^\delta \frac{dx}{k_\delta (h)}} + \frac{\delta}{\int_0^\delta \frac{dx}{k_\delta (h)}}.$$

Here $k(h)$, $k_\delta (h)$ are unsaturated soil permeability in Ω_2 and Ω_0, respectively, h_a – pressure head equivalent to the moisture on the top boundary of the contact between boundary layer Ω_0 and atmosphere. Depending on the unknown functions of the moisture transfer model, the conditions above can be transformed into analogical conditions for soil moisture or saturation.

3.3. Karstic processes on the 'salt layer–soil' interface

In this case, Ω_1 is a layer of soluble salts, Ω_2 – soil fully saturated with water, and Ω_0 – a thin boundary layer in the neighborhood of the salt dissolution front. Existence of such layer is justified in [18] and its impact is studied in [19]. The presence of a diffusion layer is also studied in [20] concerning the contaminant transfer problem. According to Fick's law, as in (6), the conjugation condition for the salt concentration is

$$D\left(c,T\right)\left.\frac{\partial c}{\partial x}\right|_{x=0\pm}=-\frac{c^{+}-c^{-}}{\int_0^\delta\frac{dx}{D_\delta(c,T)}}.$$

Here D and D_δ are diffusion coefficients of the soluble salts with concentration c, which also nonlinearly depend on temperature. Concentration c^- in this case in known and equals to the maximum saturation C_m. Concentration c^+ is an unknown concenration c on the soil surface. Then, using the congugation condition, we can write the following balance boundary condition:

$$D\left(c,T\right)\left.\frac{\partial c}{\partial x}\right|_{x=0}=-\frac{c|_{x=0}-C_m}{\int_0^\delta\frac{dx}{D_\delta(c,T)}}. \tag{9}$$

In case $D_\delta\left(c,T\right)=D_\delta=const$, similar to (8), from (9) we get

$$D\left(c,T\right)\left.\frac{\partial c}{\partial x}\right|_{x=0}=-D_\delta\frac{c|_{x=0}-C_m}{\delta}. \tag{10}$$

Condition (10) conforms with the balance boundary condition on the edge of dissolution front derived through other reasoning [18]. However, condition (9) allows for variation of diffusion coefficient on the thin boundary layer. The method of deriving conditions (9) and (10) suggests that it is a special case of a more general condition – the conjugation condition for a thin inclusion.

3.4. Balance boundary condition for the diffusion of carbon dioxide from the soil to the atmosphere in the presence of thin boundary layer

According to the model of CO_2 diffusion [21], by analogy with (9) we can derive

$$D\left(c,T,h\right)\left.\frac{\partial c}{\partial x}\right|_{x=0}=-\frac{c|_{x=0}-c_a}{\int_0^\delta\frac{dx}{D_\delta(c,T,h)}}.$$

Here c is concentration of carbon dioxide in the soil, c_a – concentration of carbon dioxide on the contact of boundary layer and atmosphere, $D(c, T)$ and $D_\delta(c, T, h)$ – diffusion coefficients of CO_2 in the soil and boundary layer, respectively.

Note that similar conditions, diverging only in numerical values of parameters, can be used for the processes of greenhouse gas distribution from the surface of a waste storage covered with geobarrier or from a surface of constructed wetland with a thin layer of water.

4. Conclusions

Conjugation conditions are integral parts of boundary-value problems for partial differential equations as mathematical models of processes in environments with thin inclusions. In this work, we have demonstrated how the balance boundary conditions can be derived as modified conjugation conditions when geobarrier is located at the boundary of problem domain instead of its interior. This is similar to a way two-phase Stefan problem is transitioned to one-phase problem. On example of a dissolution in the 'salt layer-soil' interface, we have shown that the problems with thin inclusions and boundary layers belong to the same class of problems.

The methodology of deriving these boundary conditions, proposed in this work, allows to take into consideration dependencies of the process parameters along the thickness of the boundary layer. As to the problems with modified conjugation conditions, as described in the proposed methodology, it is demonstrated that significant differences in predictive calculations might arise as compared to the classical conjugation conditions [17, 13, 10, 11]. Our further research will concern numerical experiments and analysis of the influence of these effects on the problems with thin boundary layers.

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