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RELIABILITY OF MODELS FOR SEEPAGE FLOW WITH RESPECT TO CORRECT FORMULATION OF BOUNDARY PROBLEM

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Abstract. Some groundwater flow models even commercially successful meet troubles at pratical application in complex and large aquifers with free surface. Part of them origin from lack of information on input data, other stem from model properties as consequence of particular simplification of flow phenomena. The paper deals with the second group. Namely with the problem of free boundary. Reasons and nature of the most frequent problems and limitation their in use are treated there from hydrodynamic point of view. It is shown, that a possible way out leads through the well posed boundary problem only. The paper also presents some basic information on the effective model systems INKANS and SKOKY being built up on correct solution of these problems. The solution arises from methodological possibilities of the hydrodynamic theory of boundaries (Kosorin 1983, 1993) and directly relates to solution of the problem of unknown moving boundary of flow.Both models have been successfuly applied to various simulation tasks, e.g. INKANS to the 3-D groundwater dynamics in large aquifer with complex interaction with channel and river system. 3-D pressure and velocity fields in domains with flow singularities were simulated by SKOKY. Several application samples are presented in grafical form.

Key words: Model Reliability and Limitations, Hydrodynamic Theory of Boundaries, Free Surface Flow, Well Posed Boundary Conditions, Free Boundary problems, Hydrodynamics Theory of Boundaries, Velocity Jump Relations.

I. Introduction. The problem of free (moving) boundary occurs when the model domain has a free surface of water and such flow patern, which does not allow any simplifying e.g. by shallow water theory assumptions leading to the Boussinesq type of model. Boundary condition on free surface is nonlinear and moreover it contains additional unknown (free surface position) of the model. Since this condition is unplesant, many standard and commercialy successful model systems do not respect it, e.g. MODFLOW, MIKE SHE and others, see (Mc Donald and Harbaugh 1988) and (Refsgaard et all. 1995). But, of course, such avoiding this problem usualy brings troubles with computational accuracy, (see e.g. (Refsgaard et all. 1995), because this boundary condition guarantees the mass conservation in model computations.

Strongly nonhomogeneous and layered aquifer also require specific approach due to discontinuities in velocity field. Nevertheless, this problem can be overcome by proper use of standard computational methods. I. Kazda in [1] gives suitable example for groundwater flow simulation in multilayered rock continuum by such a way.

Since some mentioned problem and their solution have use in the mathematical model building in hydrogeology, the proper source of arguments and terminology for next treatment has been taken from the book by Rushton and Redshaw [7].

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II. Well posed boundary problem as necessary condition for mathematical and numerical model to be correct

II.1 Confined aquifer. Substituting the velocity vector **q** in the mass conservation equation

$$\frac{\partial \rho}{\partial t} + div(\rho \mathbf{q}) = 0 \qquad \text{(II.1)}$$

by Darcy´s relations and expressing the compressibility effects of the saturated volume element by means of the specific storage coefficient [m^{-1}]

$$S_s = \frac{1}{\rho}\frac{d\rho}{dP}$$

then after neglecting the non-linear terms one obtains the differential equation for the hydraulic head (potential) P[m] in the form

$$\frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial P}{\partial x_j} \right) = S_s \frac{\partial P}{\partial t} + R \qquad \text{i, j = 1, 2, 3} \qquad \text{(II.2)}$$

where x and t are the space and time variable, K is the hydraulic conductivity tensor [ms^{-1}] and the sink/source term R[s^{-1}] expresses the specific outer inflow/outflow (m^3s^{-1}/m^3).

It should be said, that (II.2) has the same form as it written in [6] (appendix A1-7) as well as in [7] (eq. 2.9 on p.16). Eq. II.1 applies on the whole domain between impermeable base of aquifer ∂G_1 z=h_0(x,y) and impermeable top of aquifer ∂G_2 z=h(x,y) as the material boundaries. The boundaries ∂ G of G are completed by so-called geometrical (usually vertical) boundaries ∂ G_3 conjoining the h_0 with h.

Boundary problem for domain G is formulated by eq. II.2 and the set of boundary conditions as follow (n is the normal to boundary):

- in whole G the eq. (II.2) invalid (II.3)

- on $\partial G_1\, \partial P / \partial n = 0$ (zero normal flux) (II.4)

- on $\partial G_2\, \partial P / \partial n = 0$ (zero normal flux) (II.5)

- on ∂G_3 the normal flux or P is given (II.6)

There is also need to say that all boundaries ∂ G in set (II.3) to (II.6) are known (given). Now it is important, that the boundary problem given by the set (II.2) - (II.6) is well posed - in sense of uniqueness theorem (unique solution of the problem). Therefore, only numerical model based on an appropriate solution of the above boundary problem can always yields“ good results for good input data”.

II.2 Unconfined aquifer. The Unconfined aquifer differs from the confined by physical nature of the upper boundary ∂G_2 what is now the free surface (water table). Ofcourse, this difference is crucial and has to be accepted in the boundary conditions formulation. Namely, instead of one condition (II.5) there is need to set two conditions on $\partial G_2 \left(z = h(x, y, t)\right)$:

$$P = h \quad \text{and} \quad \partial P / \partial n = -V_n / K_n \quad \text{on} \quad z = h \qquad \text{(II.7)}$$

where V_n is the normal velocity component of the moving boundary h(x,z,t). The dynamic condition P = h arises from constant (atmospheric) pressure and the kinematic condition $\partial P / \partial n = -V_n / K_n$ represents the important mass conservation law on the free water surface.

Writing the second condition in (II.7) explicitly one obtains:

$$P = h; \; S_Y h_t + \overline{u} h_x + \overline{v} h_y - \overline{w} = 0 \qquad \text{on} \qquad z = h \qquad \text{(II.8)}$$

where S_Y is effective porosity (specific yield), $\left(\overline{u}, \overline{v}, \overline{w}\right)$ - the boundary velocity vector and (h_t, h_x, h_y) are the partial derivatives of the function h(x,z,t).

The boundary problem for unconfined aquifer is well posed by (II.1)- (II.6) only if (II.8) is written instead of (II.5). Therefore any mathematical and numerical model of groundwater flow in unconfined aquifer has to accept both conditions in (II.8) in order to be hydrodynamically correct and to yield reliable results. The reason is simple. The conditions P = h on ∂G_2 alone is not sufficient, because now the position h is unknown (added dependent variable of the problem).

Above formulation of the boundary problem for domain with free boundary is known very well and agrees also with analysis in [7], (except differences in formal approach, see pp.5 - 21). Inspite that there occur simulation models (MODFLOW, MIKE SHE, for example), based on ill posed boundary problem without the second (kinematic) condition in (II.8). Here is origin of troubles with the model validation and namely with model precision, see [6], vol. 2, p.p. 5-18 and 5 - 54.

II.3 On compressibility effect in unconfined aquifer. The free boundary problem here is unpleasant because of its nonlinearity. For unsteady flow it seems alluring to avoid the problem assuming a possibility to determine the unknown boundary h(x,y,t) only from the basic eq. (II.2) and the first eq. P = h in (II.7). Incorrectness of such proceeding can be illustrated by comparison of two effects - the aquifer compressibility and the specific yield due to free water surface movement.

Let us introduce the substitution

$$P = h + \varepsilon \; (x,y,z,t) \qquad \text{(II.9)}$$

and integrate the eq. (II.2.) along water depth $H = h-h_0$. If we apply the kinematic condition of (II.8) and the rule on differentiation of definite integrals with respect to a parameter, then we obtain

$$\frac{\partial}{\partial x}\left(K_x H\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y H\frac{\partial h}{\partial y}\right)=\left(HS_s+S_y\right)\frac{\partial h}{\partial t}+RH+F(\varepsilon) \qquad \text{(II.10)}$$

what for small ε represents the known Boussinesq eq. (satisfying the Dupuit-Boussinesq assumptions). The specific storage S_s is within the range 10^{-5} to 10^{-7} [m^{-1}], see [7], p. 19. The porosity S_y is in the range 0.1 to 0.6. Since the value of HS_s for H<1000 m is always less than 10^{-2}, eq. (II.10) indicates, that movement of the free surface yields a more water than the quantity due to the compressibility effects. Therefore the specific storage can be neglected and the differential equations quoted above in the form for steady-state problems can be used.

This statements agrees with those in [7] on p. 19. Moreover, because for the stationary problems the term with S_s in basic differential eq. vanishes, the effect of the pore volume compressibility and the water compressibility has very small domain to be used. It is for groundwater flow with free surface only if the water depth H of aquifer overtops 1000 m. On the other hand simulation models ignoring the kinematic boundary conditions in (II.8) open question on theirs reliability regardless the specific storage effect consideration.

III. Boundary problem formulation in the models INKANS and SKOKY.

Certainly it is possible to solve correctly the above problems and to build up corresponding simulation models on base of the finite element, finite differences as well as the boundary elements methods. Nevertheles, the next treatment introduces some information on building the model system of desired properties independently on the standard methods above mentioned.

The three-dimensional numerical simulation models of seepage flow INKANS and SKOKY are based on the mathematical model, consisting of equations

$$\text{grad } P + \mathbf{q}/\mathbf{k} = 0, \qquad \text{(III.1)}$$

$$\text{div } \mathbf{q} = 0 \qquad \text{(III.2)}$$

for the pressure function (potencial) P = z + p/g + const and three components of the velocity vector q, where p is the hydrodynamic pressure and z is the vertical space variable (in direction of the gravitational acceleration g). Model is completed with correctly stated boundary conditions including that for free surface. To avoid an uncertainity in computational accuracy the requirement to have a well posed boundary problem has been satisfied always for the both models.

Comprehensive formal mathematical decription of solution of the formulated boundary problem by means of the hydrodynamic theory of boundaries is presented in [2], [3] and [4]. Therefore only some methodical aspects and consequences of the solution are treated here. This solution is closely and directly connected with the solution of the problem of unknown moving boundary, which is in our case the free surface z = h(x,y,t).

The key to solution of both problems is the possibility to transform each three-dimensional boundary problem for (III.1), (III.2) over the whole domain below the free surface h(x,z,t) into a two-dimensional one for this boundary. Kosorin in [4] demonstrated the possibility and process of this transformation, including its hydrodynamic (physical) interpretation. The first step of the transformation yields the 3-D velocity field

$$q(u,w,v) = F(H, h_t, h_x, h_y, h_{xt}, h_{yt}, h_{xx}, h_{yy}., z) \tag{III.3}$$

in form of the Taylor′s series for velocity components u,v,w in the direction of y between h(x,y,t) and impermeable boundary $h_0(x,y)$. Eq. (III.3) in actual explicit form has been derived in [4] using the concept of inner and outer partial derivatives on material boundary of flow. To complete the simulation numerical model it is sufficient to operate with the equation of mass conservation for horizontal streams Φ,Ψ, the saturated depth of the porous medium $H = h-h_0$ and the porosity m and to get eq.

$$mh_t + \Phi_x + \Psi_y = 0, \quad \left(\Phi = \int_{h_o}^{h} udz, \Psi = \int_{h_o}^{h} wdz \right) \tag{III.4}$$

which results from integration of the eq. (III.2) according to z between h_0 and h. Equation (III.4), after elimination of the horizontal velocity components u and w, can be transformed by mean of (III.3) into a form of the partial differential equation of the N-1 order for the free surface h(x,y,t), N>1.

The next important yield of the hydrodynamic theory of boundaries are so-called “jump relations”. Seepage velocity field in layered porous environment is discontinual, i.e. going through layer interface it overcoms a jump. Three jump relations between velocity components in front of and behind the interface follow from (III.1) and (III.2) using the formal relations among inner and outer derivatives of potential P on interfaces, see (Kosorin 1993). The jump relations are important for the model concept of SKOKY as well as for the numerical representation of eq. (III.3) in model INKANS.

Model INKANS is based on the numeric integration of system (III.3), (III.4) for 3-D flow with free surface. Numeric integration applies the method of mean values, by means of which the system (III.3), (III.4) has been transformed in a system of ordinary differential equations of the 1-st order each of them related to one element of domain.This system was integrated by the method of the predictor-corrector type of the 2nd order with variable time step.

Model INKANS was applied for simulation of the 3-D seepage velocity field in estimating the impact of the hydropower project Gabčíkovo on groundwater of the Danube Island Zitny ostrov, influenced by the interaction with the river Danube and with the channel network of the concerned area, see Figs. [4].

The concept of discontinual velocity field and above mentioned jump relations are base of the model SKOKY algoritm. In one element of model domain the permeability is supposed to be constant. The velocity distribution is assumed to has linear and the pressure function P quadratic distribution in the same element. Using this by means of chosen approximation function in the system (1) and (2) one obtains the first part of linear equation of the model. The second part is given by the velocity jump relation valid on the interfaces among elements. The final part of equations arises from the boundary conditions. Therefore the result scheme is implicit.

The horizontal discretization of the model domain is rectangular with nonhomogeneous size of rectangles. Interfaces of layers in vertical discretization can be nonparallel. The discontinual velocity concept and the elastic discretization of the model domain allow to apply this model for the groundwater dynamics simulation in complex domains with singularities of various kind. Some of them are seen in Figs. 1, 2, 3.

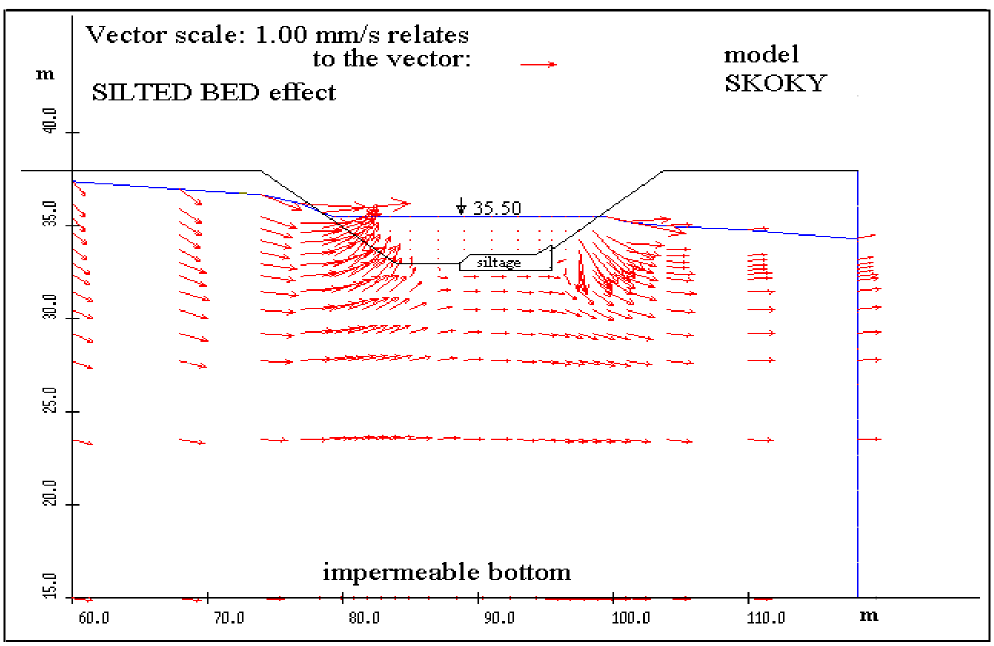

FIG. 1 *Asymetric groundwater-surface water interaction along partly silted channel bed. Simulation by model SKOKY*

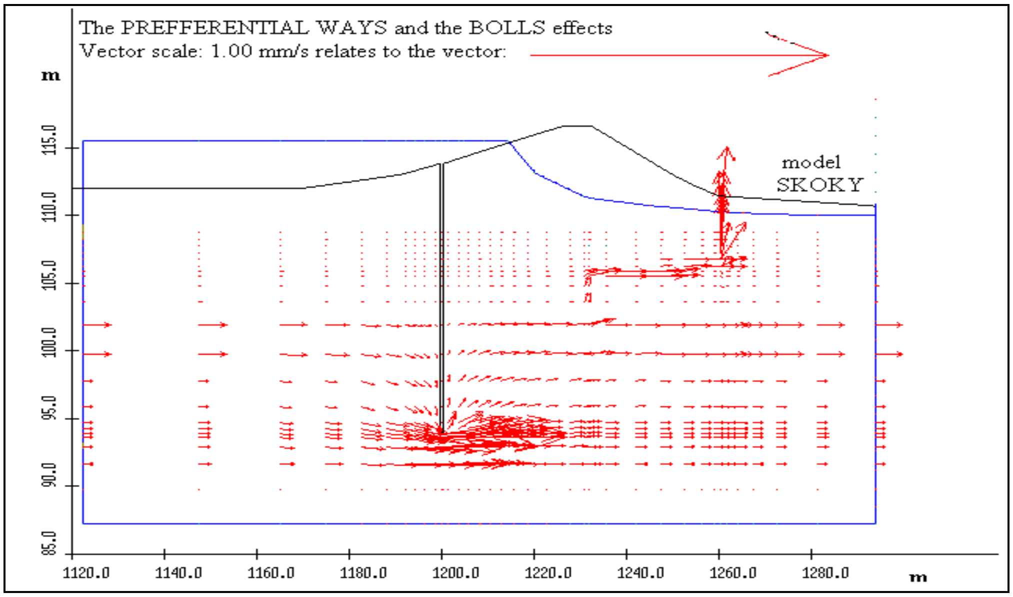

FIG. 2 *By-passing a sealing wall below dike. The preferential ways and the boil effects. Velocity field. Model SKOKY*

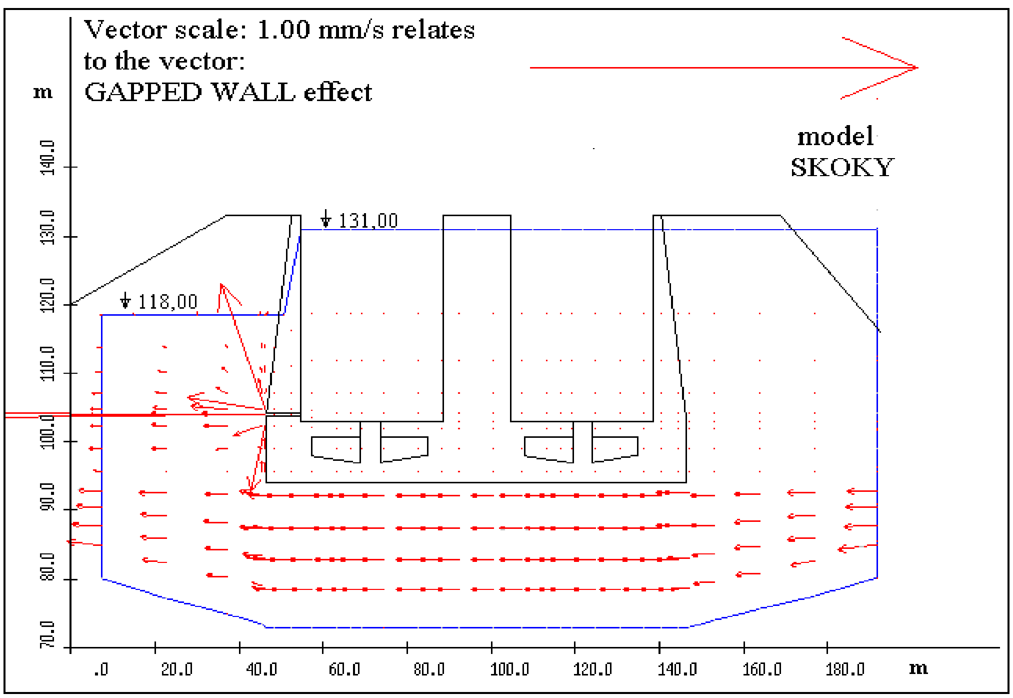

FIG. 3 *Groundwater flow around navigation lock chamber with left wall gapped; leakage effect; velocity field. Model SKOKY*

IV. Conclusion. The analysis in chapter 2 implies that the effect of the pore volume compressibility and the water compressibility has very small domain to be used. For the groundwater flow with free surface it should be only if the water depth H of aquifer overtops 1000 m. On the other hand, if the simulation model ignores the kinematic boundary conditioin in (II.8), then it open question on its reliability regardless of the specific storage effect consideration.

The algorithm of the model system INKANS and SKOKY solves the problem of free boundary utilising a possibility to transform the given boundary problem from the originally N-dimensional domain into problem, defined upon its N-1 dimensional boundaries. The crucial fact allowing this transformation is, that knowledge of the shape and motion of the free surface of seepage flow is sufficient to describe the velocity field below this surface**.** The next important property is the possibility to consider the discontinual velocity field and to use the obtained velocity jump relations.

Model INKANS has been applied to simulate the influence of the Gabcikovo reservoir filling on the groundwater dynamics of the 1450 km^2 Zitny ostrov aquifer. Simulated movement of the free water surface shows very good accordance with field observations, see [4].

Model SKOKY can be used as solitary as well as submodel of INKANS for local scale simulations. Its recent applications on the groundwater dynamics in domains with flow singularities including leakage, preferential ways, boils and other effects show real possibility to utilize it for special tasks, e.g. for the localization of gaps in underground structures or preferential ways in leve‘e and dam body.

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