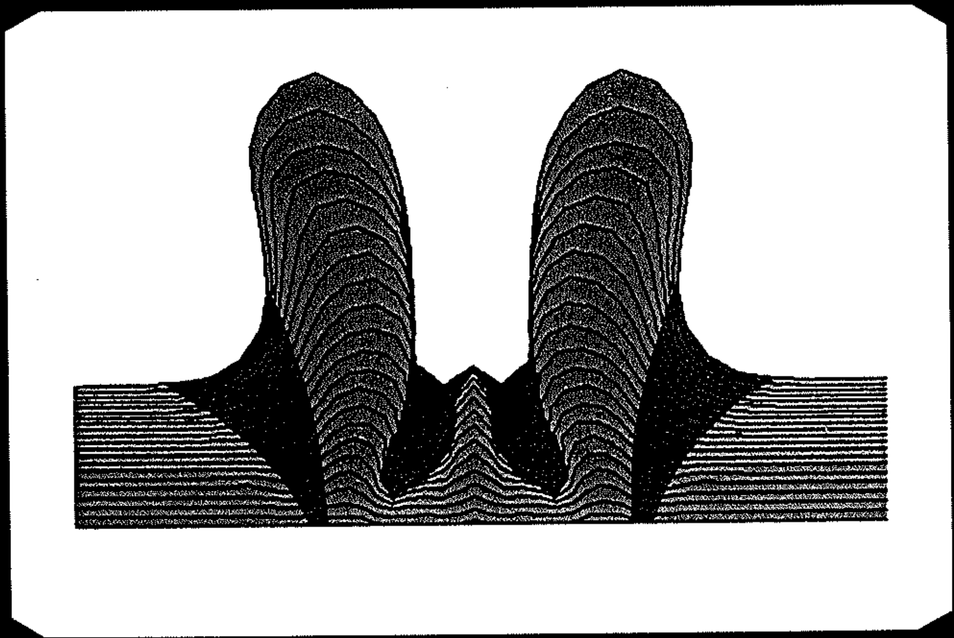
Computational Modelling of Free and Moving Boundary Problems II

Editors: L.C. Wrobel and C.A. Brebbia



Computational Mechanics Publications

Computational Modelling of Free and Moving

Editors: L.C. Wrobel and C.A. Brebbia

Transient simulation of water table aquifers using a pressure dependent storage law

A. Dassargues

Laboratoires de Géologie de l'Ingénieur, d'Hydrogéologie, et de Prospection Géophysique (L.G.I.H.), University of Liège Bat. B19, 4000 Liège, Belgium

ABSTRACT

In groundwater problems involving unconfined aquifers, the shape and the location of the water table surface have to be determined as a part of the solution of the flow problem. The transient changes affecting the position of this free surface alter the geometry of the flow system so that the relationship between changes at boundaries and changes in piezometric heads and flows must be non linear. Methods have been developed recently using fixed mesh grids and non linear codes. They are based generally on non linear variation laws of the hydraulic conductivity of the porous medium in function of the pore pressure.

Other methods based on the variation of the storage are exposed. When coupled with the hydraulic conductivity variation law, they lead to solving the generalised well-known Richards equation described and used by many authors to simulate the unsaturated flow. Considering here only the saturated flow, different relations based on arctangent and polynomial functions, linking the storage of the porous medium to the water pressure are proposed in order to reach a very good accuracy in the determination of the water table surface which is the moving boundary of the saturated domain.

DEFINITION AND CONDITIONS CHARACTERIZING A WATER TABLE SURFACE

The water table surface of an unconfined (or water table) aquifer is defined as the locus where the macroscopic pore pressure is equal to the atmospheric pressure. However, above this surface, moisture does occupy a part of the pore space. The shape and the location of the water table surface have to be determined as a part of the solution of the flow problem. Two conditions express the definition of a free surface [1] : (1) the pore pressure p is equal to zero (or atmospheric pressure):

$p = 0$ and $h = z$ with h = piezometric head (1)

(2) except recharge or evaporation, no flux across the free surface is considered, corresponding to a prescribed flux boundary :

$\partial h/\partial n = f$ where f is the flux (negative if evaporation) (2)

FLOW EQUATION IN CONFINED AND UNCONFINED AQUIFERS

Adding the Darcy law to the continuity equation expressing the mass conservation, the well-known equation describing the transient flow in a saturated porous medium is written (in term of pore presure p):

$$div\left[\underline{\underline{K}}.(\underline{grad}\,p+\rho.g.\underline{grad}\,z)\right]=S_s.(\partial p/\partial t) \tag{3}$$

where $\underline{\underline{K}}$ is the tensor of the permeability coefficients, ρ is the mass per unit volume of water, z is the elevation above a reference level, and S_s is the specific storage coefficient of a saturated porous medium. It characterizes the aquifer capacity to store or release a volume of water in function of the pore pressure in the formation. Considering the classical assumptions of non-compressible flows [2], it can be written:

$$S_s=\rho.g.(\alpha+n.\beta) \tag{4}$$

where α is the volumetric compressibility coefficient of the porous medium and β is the water compressibility coefficient. The coupling between the transient flow and the consolidation process is shown as the specific storage coefficient is expressed in function of the compressibility coefficients of the porous medium and water.

Usually, a storage coefficient is defined as the vertical integration of the specific storage coefficient on the thickness of the confined aquifer. It corresponds to the water volume stored or expelled per surface unit of the aquifer and per unit variation in piezometric head. For a water table aquifer, the variation of the piezometric heads induces the motion of the free surface, increasing or decreasing the amount of stored water by saturation or drainage of the porous medium. Consequently, in these conditions , the water storage per unit variation of piezometric head is mainly depending of the effective porosity. The storage coefficient of a water table is then defined by :

$$S_{coeff}=n_e+\int_{z_1}^{h}S_s.dz \tag{5}$$

where S_s is the specific storage coefficient in saturated (confined) conditions. In practice, the second term of this equation (5) is often neglected as 0.03 to 0.35 is a current range for n_e values in aquifers, whereas S_s reaches rarely values upper than 10^{-4} (m^{-1}). Although a same definition, the storage coefficients of confined and unconfined aquifers correspond mainly to largely different physical processes: drainage in water table aquifer and expulsion of water in confined aquifer for any decrease in piezometric head . The equation of the flow in a water table aquifer, is very often written considering the integration on the saturated thickness of the aquifer. By this way, the $\partial h/\partial z$ terms vanish, and all the vertical components of the flow are neglected :

$$div\left[\left(\int_{z_1}^{h}\underline{\underline{K}}.dz\right)\underline{grad}\,h\right]=n_e.\frac{\partial h}{\partial t} \tag{6}$$

In some cases of intensive water withdrawal, a confined aquifer may become a free or water table aquifer by lowering the piezometric head under the top of the upperlying aquitard. In such particular conditions, the storage coefficient passes from its confined value to the value of the effective porosity (n_e) ; there is a discontinuity.

METHODS USUALLY APPLIED WITH F.E.M. PROGRAMS

In transient conditions, the position of the water table can change significantly from its initial position, the geometry of the flow domain is altered so that the relationship between changes at boundaries and changes in piezometric heads and flows must be non linear [1]. The classical way to linearize this problem starts with a first estimation of the free surface position giving the initial boundary of the saturated domain. The piezometric heads are prescribed ($h = z$) on it. In each time step, after a first integration of the equation, the value of the computed flux $K(\partial h/\partial n)$ across the free surface is compared to the f value of equation (2). If the flow conditions are not satisfied (to a specified tolerance), the position of the free surface is adjusted in the desired direction and the problem is solved again and again, until the free surface flow conditions are met. For one time step, this "internal" process may need many adjustments (cycles) of the new position of the free surface, especially in geometrically complex cases or if the initial position has been roughly estimated. Most often, assuming the Dupuit approximation, the mesh is not changed at each cycle, but the value of the transmissivity (which is defined as the permeability coefficient integrated vertically on the saturated thickness), is actualized using the new piezometric head corresponding to the adjusted water table surface. For the computations, this change modifies the rigidity matrix, so that at each cycle a new problem is solved numerically.

Another current technique using the Finite Element Method consists in discretizing only the water saturated domain according to an initial free surface. The flow problem is solved and similarly to the first method described above, the computed value of the flux across the free surface is compared to the admitted value and its position is eventually adjusted. Here, the Finite Element mesh has to follow this moving. A new mesh is established at each "internal" iteration. As the discretization is changed, the solution of a new equation system must be found. To keep the effort to a minimum, only the geometric locations of the nodal points near the free surface are adjusted. If the mesh adjustments are made by an automatic meshing procedure, some distorted finite elements could appear in this zone, increasing the risk of instability or non-convergence in the numerical computations.

Methods, based mainly on the works of Bathe and Khoshgoftaar [3], have been developed using non linear laws. One of these methods is based on a variation law of the permeability coefficient (non linearity of K). The water table surface is not really considered as a boundary but as a particular zone where the porous medium is passing continuously from the saturated state to the unsaturated state or vice-versa. Looking in details at this zone, and considering in a first step the particular case of hydrostatic conditions, the medium is partly saturated above the water table surface. Water occupies a part of the voids (the rest being filled with air) and constitutes the wetting fluid [4]. The pressure of the water phase is smaller than the atmospheric pressure. This negative pressure reaches the capillary pressure (p_c) for the suction head value ($h=\psi$). In transient conditions, a tremendous simplification of the flow problem is achieved assuming that the partly saturated zone is translated together with the free surface [4]. This assumption can be accepted if the changes of the free surface are considered sufficiently slow that the partly saturated zone can adapt itself instantaneously to the new position of the water table. According to Vachaud [5], this requirement is as more verified as the ratio ψ/z_{sat} is lower than 1.0 (i.e. $\psi << z_{sat}$)

where z_{sat} is the saturated thickness in the aquifer. As mentioned by Dysli and Rybisar [6], from an hydrogeological point of view, the unsaturated zone can be characterized by a relationship linking the permeability coefficient to the suction pressure. To simulate the flow conditions in this zone, a permeability coefficient varying with the saturation conditions must be used [5,...].

As the curves of water content in function of the suction pressure can show quite different behaviours for the different geological media, different relationships between *K* and the pore pressure (*p*) can be chosen depending on the nature of the studied porous medium. Numerically, the permeability coefficient can be introduced as a function of the pore pressure. Empirical relations are used and experimentally adjusted in each case. Moreover the relation *K(h)* or *K(p)* is affected by hysteresis phenomena according to whether the porous medium is in drainage conditions or in wetting conditions, and according to whether the drainage or wetting processes are fully or partly completed before an inversion of the process. This capillary hysteresis, is usually not taken into account in the flow analysis [7].

Considering the 3D simulations of highly heterogeneous regional aquifers, the techniques described above are certainly not efficient. They are rejected because we really need a 3D approach (without Dupuit assumption), and because of the complexity of the meshing network. Consequently, a non linear method based on the introduction of non linear variations of the storage is presented hereafter.

METHOD USING THE NON-LINEARITY OF THE STORAGE

A variation of the water storage can also be introduced in the non linear code, as a function of the pore pressure. The method has been imagined [8] from the modelling by "enthalpic technique" of the phase changes in heat conduction problems : the phase changes occur at constant temperature, with heat storage [9]. In our case, the geological porous medium passes from unsaturated to saturated state at a constant zero pressure with storage of water. This storage corresponds mainly to the effective porosity of the medium. The obtained storage law is largely discontinuous (Fig. 1), the magnitude of the discontinuity being equal to the effective porosity of the medium.

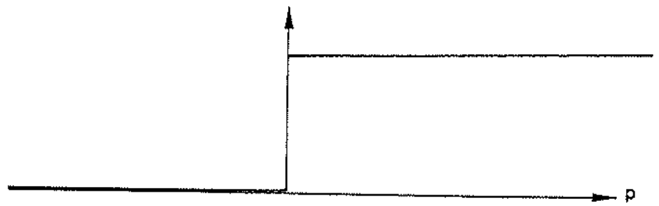


Fig. 1 Discontinuous storage law obtained by analogy to the heat storage law in thermic phase changes.

In reality, looking at the unsaturated flow with more accuracy, Musy and Soutter [7] mentioned that the well known Richards equation can be written :

$$div\left(\underline{\underline{K}}(h).\underline{grad h}\right) = -c(h).(\partial h/\partial t) \quad (7)$$

where the coefficient *c(h)* is called the capillary capacity in m^{-1}, with *h* taking negative values in the unsaturated zone and the permeability coefficient depending of *h* (cfr above). The capillary capacity of the porous medium is defined as the variation of the water content per unit variation of the negative piezometric head in the unsaturated zone. In fact, *c(h)* is completely equivalent in definition and units to the specific storage coefficient in the saturated part (Fig. 2). So that we could "generalize" the term of specific storage coefficient in both unsaturated and saturated zones. In the saturated zone S_s is constant (if the effects of the consolidation are disregarded at this stage), and in the unsaturated zone $S_s(h)$ is highly variable (Fig. 2):

$$c(h) = S_s(h) = (\partial\theta/\partial h) \text{ with } \theta \text{ the water content in the unsaturated zone} \quad (8)$$

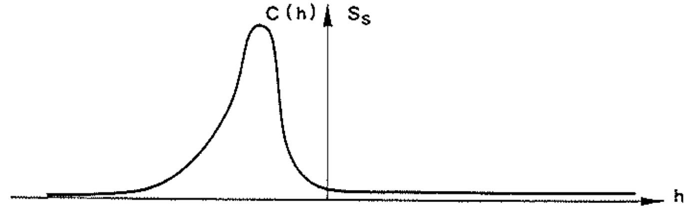


Fig. 2 Evolution of the "generalized" specific storage coefficient in both unsaturated and saturated zones, in function of *h*.

The variation of the water content per unit variation of the piezometric head in the unsaturated zone is equal to the variation of the storage (*S*) for the same variation of negative piezometric head (Fig. 3):

$$\partial\theta/\partial h = \partial S/\partial h \quad (9)$$

The relation *S(h)* can also be drawn in function of the pore pressure *p* (Fig. 4). For sandy and clayey materials the relations obtained experimentally are very contrasted, and a very abrupt decrease of the storage is observed in sandy layers when the pore pressure passes from 0 to -10 kPa (Fig. 4). In this last case, the curves can be drawn in (*log p . S*) or (*ln p . S*) diagrams. From equation (9), we obtain the relation:

$$\theta = S + \text{constant} \quad (10)$$

where the constant is equal to the water content corresponding to the residual saturation degree. This constant is less important for sandy aquifers than for clayey layers. However, this relation between *S* and *p* (or *h*) is affected by hysteresis phenomena, as exposed by Musy and Soutter [7]. In practice, as mentioned above, this capillary hysteresis is rarely explicitly taken into consideration in flow analysis.

Numerically, a variation law of the storage can be chosen on basis of experimental data, and implemented in the non linear code. That can be a polynomial or an arctangent function, but the main stumbling-block consists in finding a sufficiently relaxed storage law in order to avoid any numerical overflow in the F.E.M. computations. The variation of the storage in the unsaturated zone can be described, for example, by a polynomial function of the following type (Fig. 5) :

$$S(p) = n_e.\left[C_0 + C_1(p/-a) + C_2(p/-a)^2 + C_3(p/-a)^3 + C_4(p/-a)^4\right] \quad (11)$$

with the prescribed conditions: (1) $S(p) = 0$ or Cst if $p = -a$

(2) $S(p) = n_e$ if $p = 0$

(3) $dS(p)/dp = 0$ if $p = -a$

(4) $dS(p)/dp = 0$ or $S_s/\rho.g$ if $p = 0$

(5) $d^2S(p)/dp^2 = 0$ if $p = -2a/3$

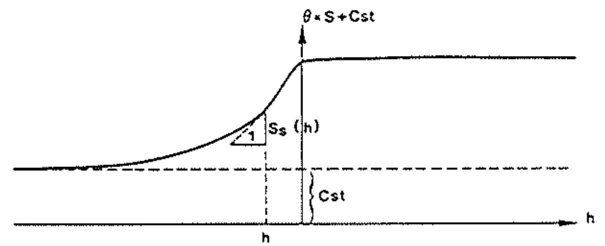


Fig. 3 Evolution of the water content and of the storage in both unsaturated and saturated zones, in function of h.

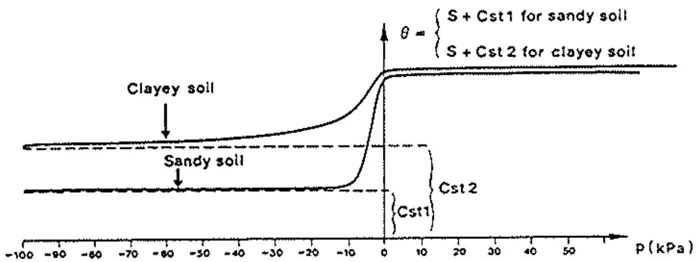


Fig. 4 Evolution of the water content and of the storage in function of p, for sandy and clayey soils.

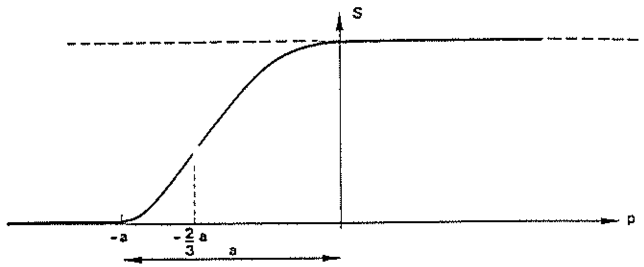


Fig. 5 Polynomial storage law in the unsaturated zone, the location of the inflexion point can be prescribed.

The conditions (1) and (3) express that at a given negative pressure ($p=-a$), we approximate the storage value by a constant (or zero) and its variation in function of the pressure (its derivative) by zero values. Similarly the conditions (2) and (4) express that at the atmospheric pressure ($p=0$), we consider that the storage has reached a constant value equal to the effective porosity and its derivative is equal to zero (as we neglect the specific storage coefficient of saturated conditions in front of the effective porosity, cfr above). The condition (5) prescribes the location of the inflexion point in

the polynomial curve that we try to fit to the experimental data. In the case of the Fig. 5, this location has been chosen at $p = -2a/3$. The five constants of the equation (11) are calculated using the five equations provided by the five prescribed conditions. The expression of the storage law in function of the pore pressure becomes in our case:

$$S(p) = 0 \quad \text{for} \quad p < -a$$

$$S(p) = n_e.\left[1 - 4(p/-a)^3 + (p/-a)^4\right] \quad \text{for} \quad -a \le p \le 0 \tag{12}$$

$$S(p) = n_e \quad \text{for} \quad p > 0$$

The degree of the polynomial function and the different conditions are found on basis of experimental data about the water content in the unsaturated porous medium.

APPLICATIONS AND PROSPECT FOR FUTURE WORKS

Our non-linear code, called LAGAMINE [2,10], has been already used to model in 3D different regional water table aquifers with a high level of accuracy: (a) the groundwater model of a regional water table aquifer, called "Hesbaye aquifer", in Belgium [10]; (b) the regional groundwater model of an alluvial water table aquifer in the valley of the Meuse River downstream to the city of Liège (Belgium) [11]: For these studies, the complexity of the geological conditions, the 3D discretization, the required accuracy added to the transient conditions, have justified fully the use of the Finite Element Method with a fixed meshing network and using a non linear storage law. Unfortunately, no accurate data were available concerning the water content or storage variation in the unsaturated porous media of both cases (the fissured chalk in the "Hesbaye aquifer" and the fluviatile deposits in the River Meuse alluvial aquifer). As mentioned previously by the author [12], an arctangent storage law has been used to approximate the variation of the storage in function of the pore pressure:

$$S = n_e.\left(\frac{1}{\pi}.arctg\left[\frac{p + Cst}{\alpha_r}\right] + \frac{1}{2}\right) + \frac{S_s}{\rho.g}.\langle p \rangle \tag{13}$$

where $\langle p \rangle = p$ if $p > 0$
$\langle p \rangle = 0$ if $p \le 0$

α_r = relaxation coefficient influencing the shape of the function (Fig. 6).
Cst = constant allowing to translate the arctangent function (Fig. 6).

The storage arctangent function has been applied with $Cst=0$ and $\alpha_r = 1\ 10^4$ Pa. As the arctangent function is here a purely theoretical function, neither based on actual data, nor verified, the unsaturated flows have been excluded from the computations. After many 1D, 2D and 3D simple tests (comparisons with analytical and other numerical solutions)[10], the accuracy of the computations has been verified and the two case studies mentioned above have been completed [10,11].

In a future prospect, it would be very useful to adjust actual data on the polynomial law of the 4th degree (see above) which should be convenient to describe the storage evolution. A better approximation in the changeover zone where the medium passes from the saturated to the unsaturated state will be obtained, considering that the unsaturated flow has an influence on the saturated flow. It should be convenient in order to simulate unconfined aquifers with accuracy using F.E.M. models.

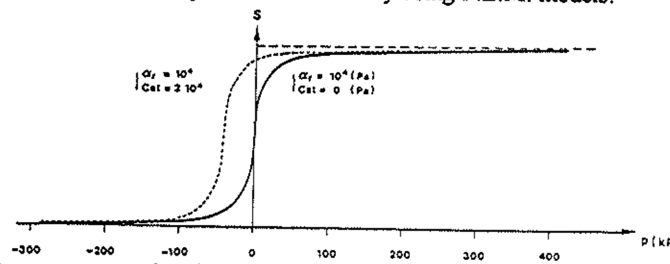


Fig. 6 Arctangent storage law in the unsaturated zone, the parameter a influences the relaxation of the curve and the constant (Cst) can translate the curve.

ACKNOWLEDGEMENTS

The numerical developments have been introduced in the Finite Element code "Lagamine" which is the research code of M.S.M. and L.G.I.H. departments of the University of Liège. Thanks to Mr J.P. Radu of the M.S.M. team for the valuable work he provided in some complex numerical situations. This research was supported by the Scientific Policy Services of the French speaking Community of Belgium. Thanks to IBM (Belgium) support, the "Lagamine" code is now running on a IBM/Risc 6000 system in the L.G.I.H. department of the University of Liège.

REFERENCES

1. Bear, J., and Verruijt, A., *Modeling groundwater flow and pollution*, Reidel, 414 p.,1987.
2. Dassargues, A., *Paramétrisation et simulation des réservoirs souterrains, Discrétisation du domaine, Préparation statistique des données, Couplages et non linéarités des paramètres*, PhD Thesis, Applied Sciences Faculty of the University of Liège,Belgium, 1991.
3. Bathe, K.J. and Khoshgoftaar, M.R. 'Finite element free surface seepage analysis without iteration', *Int. J. Num. and Anal. Meth. in Geomechanics*, Vol. 3, pp. 13-22, 1979.
4. Dagan, G., *Flow and transport in porous formations*,Springer-Verlag, 465 p.,1989.
5. Vachaud, G., *Contribution à l'étude des problèmes d'écoulement en milieu poreux non saturés*,Thèse de Doctorat, Grenoble,1968.
6. Dysli, M. and Rybisar, J. 'Coupled models and free-surface seepage analysis without mesh iteration', in ICONMIG/88 (Ed. Swoboda, G.), pp. 791-795, *Proceedings of the sixth Int.Conf.on Numerical Methods in Geomechanics*, Innsbruck, Austria, 1988.
7. Musy, A. and Soutter, M. , *Physique du sol*, Presses Polytechniques et Universitaires Romandes, Collection Gérer l'Environnement n°6, 335 p., 1991.
8. Charlier, R., Radu, J.P. and Dassargues, A. 'Numerical simulation of transient unconfined seepage problems, in Computer and Water Resources' Groundwater and aquifer modelling (Ed. Ouazar D. and Brebbia C.A.), pp. 143-155, *Proceedings of the 1st Int. Conf. in Africa on Computer Methods and Water Resources*, Vol. 1, Rabat, Morocco, 1988.
9. Comini, G.,de Guidice, S.,Lewis, R.W. and Zienkiewicz, O.C., 'Finite Element solution of non linear heat conduction problems with special reference to phase change', *Int. J. Num. Meth. in Eng.* , vol.8 , pp. 613-624, 1974.
10. Dassargues, A., Radu, J.P.and Charlier, R. 'Finite element modelling of a large water table aquifer in transient conditions', *Adv. in Water Resources*, Vol. 11, June, pp. 58-66, 1988.
11. Dassargues, A. and Lox, A. 'Modélisation mathématique de la nappe alluviale de la Meuse en aval de Liège (Belgique)', 'Le système hydrologique dans la région frontalière Liège-Maasbracht; résultats des recherches 1985-1990', *Rapport et notes* n°26 ,*CHO-TNO*, Delft, pp. 27-54.,1991.
12. Dassargues, A. 'Water table aquifers and Finite Element Method: Analysis and presentation of a case study', in Moving Boundaries/91 (Ed. Wrobel, L.C.,Brebbia, C.A.),vol.1 Fluid flow, pp.63-72, *Proceedings of the Int. Conf. on Computational Modelling of Free and Moving Boundary Problems*, Comp. Mech. Publ., 1991