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TRANC: A Modification to CORCON MOD2 for Modelling Transient Thermal Conduction in the Concrete Basemat of a Reactor

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Abstract

CORCON MOD2 uses a quasi-steady-state model for ablation in the concrete basemat. TRANC is a modification for CORCON MOD2 which uses a thermal penetration approach to model transient thermal conduction in the basemat. It also provides an interface for linking to more sophisticated models for the concrete. Example calculations are presented. The TRANC modification has been applied to CORCON 2.04.00. The new version is called CORCON 2.04.TRANC.

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1. Introduction

In the unlikely event of a severe accident in a nuclear power plant, material from the core of a reactor may come into contact with the concrete basemat. The CORCON MOD2 code [1] models the subsequent interaction. However, CORCON MOD2 is restricted to phases of the interaction where ablation of the concrete is essentially steady state. The code may not be applicable to early times before the steady state ablation rate and temperature profile have been established or at late times after steady state ablation has ceased (the code assumes zero heat flux into the concrete if there is no ablation).

This paper describes new models which have been added to CORCON MOD2 to extend its applicability. The official release CORCON2.04.00 has been used as a basis for the modifications. The new version is called CORCON2.04.TRANC.

TRANC includes a quasi-one-dimensional model for thermal conduction and ablation in the concrete basemat. The thermal conduction equation together with appropriate boundary conditions for ablation or fixed boundaries are solved using a thermal penetration approach similar to that used in INTERUK [2]. A simple model for the release of gas from the concrete is used. It is the same as the original model in the special case of steady state ablation. The models for heat transfer and crust growth in the melt have not been updated. This part of the calculation is still based on quasi-steady-state models.

Section 2 gives a description of the models which have been added in TRANC.

Section 3 describes how the new models have been interfaced to CORCON.

Two sets of example calculations are presented in Section 4:

1) Calculations for the TURC 2 [3] experiment have been performed. The initial transient conduction in the concrete is important in this

experiment. Transient phenomena in the melt may also be significant but these are not modelled.

2) Plant calculations for a hypothetical accident sequence [4] have been repeated with the new version of the code. There is little difference between CORCON2.04.00 and CORCON2.04.TRANC at medium times as was expected. The differences at early times do not have a long term effect. At late times, when ablation is expected to cease, large differences were found in one case. These were due to an instability associated with suddenly stopping heat transfer to the concrete when there was no ablation in the original code. This instability could probably be controlled by using very small time steps. Far more important differences were found between cases with different ablation temperatures for the concrete than between cases run using the different versions of the code. An ablation temperature of 1600K led to less than 1 metre of vertical penetration into the concrete. With an ablation temperature of 1420K ablation was still continuing after 10 days and the penetration exceeded 7 metres.

Details of the changes made to the code and the format of the new data set are given in appendices 3,4 and 5. The modifications have been put into UPDATE form.

2. General Description of the Models in the TRANC Modification

2.1 Analytic Formulation of the Thermal Conduction Problem in the Concrete Basemat

The situation in the reactor basemat is represented in figure 1. Axial symmetry is assumed about the line EF.

Thermal conduction is assumed to occur in the region ABCDE of the concrete:

$$\rho c \frac{\partial T}{\partial t} = \nabla . (k \nabla T) \qquad (1)$$

where $T(\underset{\sim}{x},t)$ is the temperature at position $\underset{\sim}{x}$ and time t, ρ is the density of concrete, c the specific heat of concrete and k is the thermal conductivity.

There are two types of boundary. Boundaries BC, CD, DE are exterior boundaries where interfaces with rock and soil or other parts of the containment building occur. In this paper they will be ignored by assuming that they are at infinity. The boundary conditions are then:

$$T(\underset{\sim}{x},t) \to T_\infty \quad \text{as} \quad |\underset{\sim}{x}| \to \infty \quad \text{and} \quad \underset{\sim}{x} \text{ is in the concrete} \tag{2}$$

T_∞ is the ambient temperature.

The boundary AB is an interior boundary between the concrete and the melt pool, atmosphere or coolant layer. This boundary may move with time. The boundary condition is

$$\rho L \dot{\underset{\sim}{x}}_m = \left[(\underset{\sim}{\phi} + k\nabla T|_{\underset{\sim}{x}_m}) \cdot \underset{\sim}{n} \right] \underset{\sim}{n} \tag{3}$$

— if ablating

$$T(\underset{\sim}{x}_m, t) = T_m \tag{4}$$

or

$$(\underset{\sim}{\phi} + k\nabla T) \cdot \underset{\sim}{n} \Big|_{\underset{\sim}{x}_m} = 0 \tag{5}$$

— if not ablating

$$\dot{\underset{\sim}{x}}_m = 0 \tag{6}$$

where $\underset{\sim}{x}_m(t)$ is the location of a point on the meltfront, L is the specific latent heat of melting of concrete, $\underset{\sim}{\phi}$ is the heat flux into the concrete and $\underset{\sim}{n}$ is the unit normal into the concrete. Additional constraints are required so that only one set of (3) & (4) or (5) & (6) can be applied at each point. These are:

$$\dot{\underset{\sim}{x}}_m \cdot \underset{\sim}{n} > 0 \quad \text{for ablation} \tag{7}$$

i.e. the melt front can only advance, and

$$T(\underset{\sim}{x}_m, t) < T_m \quad \text{when not ablating} \tag{8}$$

i.e. the concrete cannot be heated above its melting temperature without melting occurring.

In this work the concrete is modelled as a simple material with a fixed melting point T_m and constant specific latent heat L. However, a model where T_m and L depended on the material in the meltpool may be more realistic.

2.2 Quasi-One-Dimensional Formulation

Consider a fixed curvilinear coordinate system which is based on the location of the melt front at some fixed time t_0:

$$\underset{\sim}{x} = \underset{\sim}{x}_m (s_1, s_2) + p\underset{\sim}{n}(s_1, s_2) \tag{9}$$

$\underset{\sim}{x}_m$ is the position of a point on the melt front, s_1 and s_2 are distances along the melt front surface, $\underset{\sim}{n}$ is the normal and p is the normal distance of the point from the surface.

Then at constant time

$$d\underset{\sim}{x} = \frac{\partial \underset{\sim}{x}_m}{\partial s_1} ds_1 + \frac{\partial \underset{\sim}{x}_m}{\partial s_2} ds_2$$

$$+ p \frac{\partial \underset{\sim}{n}}{\partial s_1} ds_1 + p \frac{\partial \underset{\sim}{n}}{\partial s_2} ds_2 + \underset{\sim}{n} dp \tag{10}$$

Without loss of generality we can assume that s_1 and s_2 are measured along the principal directions of curvature then by definition,

$$\frac{\partial \underset{\sim}{x}_m}{\partial s_1} = \underset{\sim}{t}_1 \qquad (11)$$

$$\frac{\partial \underset{\sim}{x}_m}{\partial s_1} = \underset{\sim}{t}_2 \qquad (12)$$

$$\frac{\partial \underset{\sim}{n}}{\partial s_1} = \kappa_1 \underset{\sim}{t}_1 \qquad (13)$$

$$\frac{\partial \underset{\sim}{n}}{\partial s_2} = \kappa_2 \underset{\sim}{t}_2 \qquad (14)$$

where $\underset{\sim}{t}_1$ and $\underset{\sim}{t}_2$ are the unit tangent vectors in the principal directions and κ_1 and κ_2 are the principal curvatures.

Therefore

$$d\underset{\sim}{x} = (1 + \kappa_1 p)\underset{\sim}{t}_1 \, ds_1 + (1 + \kappa_2 p)\underset{\sim}{t}_2 \, ds_2 + \underset{\sim}{n} \, dp \qquad (15)$$

$\underset{\sim}{t}_1$, $\underset{\sim}{t}_2$, $\underset{\sim}{n}$ are an orthogonal set of unit vectors therefore using the standard notation for curvilinear coordinates (ξ_1, ξ_2, ξ_3)

$$h_1 = (1 + \kappa_1 p) \qquad (16)$$

$$h_2 = (1 + \kappa_2 p) \qquad (17)$$

$$h_3 = 1 \qquad (18)$$

and $\underset{\sim}{e} = \underset{\sim}{t}_1$, $\underset{\sim}{e}_2 = \underset{\sim}{t}_2$, $\underset{\sim}{e}_3 = \underset{\sim}{n}$ (19),(20),(21)

The standard formulae may be applied:

$$\nabla\psi = \sum_{i=1,2,3} \frac{1}{h_i} \frac{\partial\psi}{\partial\xi_i} \underset{\sim}{e}_i \qquad (22)$$

$$\nabla^2\psi = \frac{1}{h_1 h_2 h_3} \left(\frac{\partial}{\partial\xi_1}\left(\frac{h_2 h_3}{h_1} \frac{\partial\psi}{\partial\xi_1}\right) + \frac{\partial}{\partial\xi_2}\left(\frac{h_1 h_3}{h_2} \frac{\partial\psi}{\partial\xi}\right) + \frac{\partial}{\partial\xi_3}\left(\frac{h_1 h_2}{h_3} \frac{\partial\psi}{\partial\xi_3}\right)\right) \qquad (23)$$

substituting (16)-(18) in (23) and applying to (1) gives

$$\rho c \frac{\partial T}{\partial t} = \left(\frac{1}{(1+\kappa_1 p)(1+\kappa_2 p)}\left(\frac{\partial}{\partial s_1}\left(\frac{(1+\kappa_2 p)}{(1+\kappa_1 p)} k\frac{\partial T}{\partial s_1}\right) + \frac{\partial}{\partial s_2}\left(\frac{(1+\kappa_1 p)}{(1+\kappa_2 p)} k\frac{\partial T}{\partial s_2}\right) + \frac{\partial}{\partial p}\left((1+\kappa_1 p)(1+\kappa_2 p)\, k\frac{\partial T}{\partial p}\right)\right)\right) \qquad (24)$$

Let L_i denote the length scale over which changes in T occur in direction i, then (24) can be approximated by

$$\rho c\frac{\partial T}{\partial t} = \frac{\partial}{\partial p}\left(k\frac{\partial T}{\partial p}\right) \qquad (25)$$

provided, $L_1 \gg L_3$ (26)

$L_2 \gg L_3$ (27)

$p \ll \frac{1}{\kappa_1}$ (28)

$p \ll \frac{1}{\kappa_2}$ (29)

The boundary conditions may be approximated in a similar way. The quasi-one-dimensional approximation may be used provided that the changes in T in the normal direction are much greater than the changes in the tangential direction and that only points sufficiently close to the surface compared to the radius of curvature are considered. These requirements will be discussed later. In general terms the quasi-one-dimensional approximation applies for all points from which the melt front looks like a plane on which all quantities are uniform.

In TRANC the one- dimensional equations are set up at each point on the melt front based on the normal coordinate system at time t. These equations are then advanced to $t+\Delta t$ using the heat flux calculated by other parts of the code. This gives a distance advanced by the melt front along the normal and a new temperature profile at $t + \Delta t$.

The points on the melt front are advanced along the normals and then remapped onto the rays. The new normal coordinate system at time $t+\Delta t$ is then established and the new temperature profile is remapped onto it.

2.3 Steady State Ablation Solution

The 1-D form of the equations (1)-(8) with temperature independent thermal properties have an analytic, steady state solution for a constant heat flux ϕ ;

$$T(x,t) = T_\infty + (T_m - T_\infty)\exp(-(x-x_m)/\delta) \tag{30}$$

where

$$\dot{x}_m = \frac{\phi}{\rho(L+c(T_m-T_\infty))} \tag{31}$$

$$\delta = \frac{k(L+c(T_m-T_\infty))}{c\phi} \tag{32}$$

2.4 Thermal Penetration Approximation to One-Dimensional Ablation Problem

A Galerkin approach has been used following [2]. The basis function is

$$T = T_\infty + (T_m - T_\infty)\exp(-(x-x_m)/\delta) \tag{33}$$

where x_m and δ are functions of t. (It is capable of representing exactly the analytic steady state solution (30).)

The boundary condition is satisfied exactly:

$$\rho L\dot{x}_m = \phi - \frac{k(T_m-T_\infty)}{\delta} \tag{34}$$

The weighted residual of (1) is made zero:

$$\int_{x_m}^{\infty} \left(\rho c\dot{T} - k\frac{\partial^2 T}{\partial x^2}\right) \exp\left(-n(x-x_m)/\delta\right)dx = 0 \tag{35}$$

where n=1 represents Galerkin weighting

n=0 represents uniform weighting

Substituting (33) in (35), integrating and eliminating x_m using (34) leads to

$$\dot{\delta} = \frac{(n+1)}{\rho L}\left(\frac{k\,(L+c(T_m-T_\infty))}{c\delta} - \phi\right) \tag{36}$$

If $T_o(x)$ is the profile at t=0, δ at t=0 is determined by

$$\int_{x_m}^{\infty} (T_o - T)\exp(-n(x-x_m)/\delta)dx = 0 \tag{37}$$

2.5 Integration of Thermal Penetration Solution to the Ablation Problem

Equation (36) may be discretised explicitly:

$$\frac{\delta^n-\delta^o}{\Delta t} = \frac{(n+1)}{\rho L}\left(\frac{k(L+c(T_m-T_\infty))}{c\delta^o} - \phi^o\right) \tag{38}$$

where superscript n denotes time $t+\Delta t$, superscript o denotes time t.

It is shown in appendix 1 that for constant ϕ this scheme is stable provided

$$\Delta t < \frac{2\delta^2\rho Lc}{(n+1)k(L+c(T_m-T_\infty))} \tag{39}$$

Equation (37) may be discretised implicitly:

$$\frac{\delta^n - \delta^o}{\Delta t} = \frac{(n+1)}{\rho L} \left(\frac{k(L + c(T_m - T_\infty))}{c\delta^n} - \phi^n \right) \qquad (40)$$

This involves solving a quadratic equation. It is shown in appendix 1 that for constant ϕ this scheme is stable for all $\Delta t > 0$.

If ϕ is constant (or assumed constant) equation (36) can be integrated analytically to give t as a function of δ. This approach is not used because the resulting equation would have to be inverted using an iterative technique.

The implicit discretisation (40) is used in TRANC.

2.6 Thermal Penetration Approximation to One-Dimensional Fixed Boundary Problem

The approach is similar to the ablation problem.

The basis function is

$$T = T_\infty + (T_w - T_\infty) \exp(-x/\delta) \qquad (41)$$

where T_w and δ are functions of time.

The boundary condition (5) becomes

$$\frac{k}{\delta} (T_w - T_\infty) = \phi \qquad (42)$$

and (1) leads to

$$\rho c \dot{T}_w - \frac{k}{\delta^2}(T_w - T_\infty) + \frac{\rho c}{(n+1)} \frac{\dot{\delta}}{\delta} (T_w - T_\infty) = 0 \qquad (43)$$

If ϕ is constant this leads to

$$\dot{\delta} = \frac{k}{\rho c} \frac{(n+1)}{(n+2)} \frac{1}{\delta} \tag{44}$$

If $T_o(x)$ is the profile at $t=0$ the initial values of T_w and δ should satisfy

$$\int_0^\infty (T_o - T)\exp(-nx/\delta)dx = 0 \tag{45}$$

If there is a discontinuity in ϕ applying (42) and (45) leads to

$$\delta^+ = \frac{2(n+1)\ \phi^-/\phi^+\ \delta^-}{n+\ (n^2+4(n+1)\phi^-/\phi^+)^{1/2}} \tag{46}$$

where $^+$ denotes values at t^+, $^-$ denotes values at t^-. A discontinuity in ϕ gives a discontinuity in T_w and δ.

2.7 Integration of Thermal Penetration Solution to Fixed Boundary Problem

Assuming ϕ is piecewise constant (44) can integrated analytically:

$$\delta^n = (2(\frac{n+1}{n+2}) \frac{k}{\rho c} \Delta t + (\delta^+)^2)^{1/2} \tag{47}$$

where δ^+ is given by (46).

The accuracy of this scheme is discussed in appendix 2. It is accurate provided ϕ does not change too rapidly and it can be seen that the scheme breaks down if ϕ changes sign.

2.8 Generation of Gas From Concrete

When concrete is heated, gases are released. Evaporable water is released first between approximately 300K and 350K. Chemically constituted water is released above approximately 670K. Carbon dioxide is released above about 900K. TRANC does not model the release of gases mechanistically. It uses a simple model in which the gas release rate, $\dot{G}$ is

$$\dot{G} = f_g[(1 - f_e)\rho\dot{x}_m + f_e(\frac{\phi}{L+c(T_m - T_\infty)})] \tag{48}$$

where f_g is the mass fraction of gas released from the concrete when it is melted, starting from ambient temperature. f_e is a parameter (ER in the code) which gives enhanced gas release prior to melting. $f_e = 0$ gives no gas release before melting, $f_e > 0$ gives some release before melting but gives the same as the $f_e = 0$ case during steady state ablation.

If $T(x_m) \geqslant T_{CO_2}$ the gas release is in the same component ratios (H_2O to CO_2) as under steady state ablation. If $T(x_m) < T_{CO_2}$ only water is released.

T_{CO_2} and f_e may be varied by the user to perform scoping calculations.

3. Description of the Interface of TRANC to CORCON

3.1 Iterative Procedure for Calculating the Melt-Concrete Heat Fluxes

At each point on the melt-concrete boundary:

$$\phi^n = \phi_f^n (T_A^n, T_w^n, \dot{G}^n) \tag{49}$$

$$T_w^n = T_w^n (\phi^n) \tag{50}$$

$$\phi_P^n (T_A^n) = \phi_f^n (T_A^n, T_w^n, \dot{G}^n) \tag{51}$$

$$\dot{G}^n = \dot{G}^n(T_w^n, \phi^n) \tag{52}$$

where

Y denotes some physical quantity and Y(...) denotes a function which is equal to Y. ϕ is the heat flux into the concrete, ϕ_f is the heat flux across the gas film between the melt and the concrete, ϕ_p is the heat flux from the meltpool, T_A is the temperature of the melt - pool-film interface, T_w is the temperature of the film - concrete interface and $\dot{G}$ is the gas generation rate.

Superscript n denotes quantities that are evaluated at the new time level $t + \Delta t$. There is also an implied dependence on quantities at the old time in (49) - (52).

Equations (49) to (52) are solved in nested iterations in QWALL, SURFEB and FILM. Note that in TRANC the time step is available when FILM is called because TIMSTEP has been moved earlier in the calling sequence.

QWALL solves (49) and (50) by varying ϕ^n. This gives

$$\phi_f^n\ (T_A{}^n,\ \dot{G}^n) \text{ and } T_w^n\ (T_A^n,\ \dot{G}^n).$$

SURFEB solves (51) by calling QWALL and varying T_A^n. This gives

$$T_w^n\ (\dot{G}_n) \text{ and } \phi^n(\dot{G}_n)$$

FILM solves (52) by calling SURFEB (making (52): $\dot{G}^n = \dot{G}^n(\dot{G}^n)$) and varying $\dot{G}^n$.

3.2 Generalisation of Transport

For the steady state ablation model the heat flux into the concrete, the ablation rate, the release rates of each species of gas from the concrete and the rate at which enthalpy leaves the concrete are all proportional. The temperature of the film/concrete interface is always at the melting point of concrete. These assumptions were hardwired to a greater or lesser extent in CORCON MOD2. In the TRANC modification these restrictions no longer apply. This allows more general concrete models to be coupled to CORCON MOD2.

4 Example Calculations

4.1 TURC2 Test

The TURC2 test [3] consisted of a magnesia tube containing a concrete plug at the base. Molten urania was poured onto the concrete and the interaction was observed. In [5] preliminary calculations were performed for this experiment using CORCON 2.00.00 and INTERUK. The CORCON calculations are repeated here using essentially the same data set except for the changes specified.

Four runs have been performed. Table 1 shows the code and data used for each run together with some representative results. The other data is the same as in [5] together with data shown in table 2 (where appropriate). The radius of the cavity has been increased by a factor of 10 to give 1-D results. Figures 2, 3 and 4 show the results of runs 2, 3 and 4. It can be seen from the table and figures that the temperature of the oxide layer is similar in all cases. The main difference between cases is the vertical erosion. The erosion distances calculated when conduction in the concrete is included are consistent with the experiment where erosion was stated to be less than 5mm (cf 2mm for run 4, 1mm for run 3). A consequence of the small amount of erosion in these calculations is that little material is added to the pool and hence the solidus and liquidus temperatures remain at nearly their initial values. Figure 2 shows that there is a large discrepancy in the release of gases between cases 3 and 4. This shows the need for a transient gas release model.

The TRANC calculations do not show ablation occurring until about 500s after the start of the interaction. This differs from calculations performed in [3] where the calculations showed ablation after about 30 seconds. One reason for the difference may be the instantaneous formation of a crust in the melt in the TRANC calculations which limited the heat flux into the concrete. (The calculations in [3] were fully transient.)

In the actual experiments the debris melting point was 2600K and there was believed to be about a 100K of superheat. This is entirely different to 2820K initial debris temperature and 2830K debris melting point used in [5] and here which were based on pre-test data. Therefore no conclusions should be made from comparing the calculations with the experiment. It should also be noted that the temperatures calculated by CORCON are average layer temperatures. If CORCON predicts thick crusts the temperature of the liquid in the layer may be considerably higher.

Run No.	code version	f_e	ICOND	Vertical Penetration (mm) at t=2610s	Temperature of Oxide (K) at t=2610s
1	2.04.00	--	-	31	1586
2	2.04.TRANC	-	0	30	1586
3	2.04.TRANC	1	1	0.93	1506
4	2.04.TRANC	0	1	2.00	1483

Table 1. Calculations for TURC2 case

Radius of cavity	= 10 × real radius
Weighting parameter, n	= .752
CO_2 release temperature, TCO_2	= 1000K
Thermal conductivity of concrete k	= 2W/m/K

Table 2. Data for TURC2 calculations

4.2 Plant Calculations

Calculations similar to those performed in [4] have been repeated with TRANC. The data is appropriate to a PWR with a nominal reactor power of 3411 MW and a reactor cavity floor area of $60m^2$. The basemat consists of (by weight) 55% silica, 28% other oxides, 10% calcium hydroxide, 3% calcium carbonate and 4% free water. There is also 0.117kg of rebar steel per kg of concrete. The interaction starts with debris at 2755K (assumed to be its melting point) and 95.7% molten. Initially the debris consists of 101 tonnes of UO_2, 10.8 tonnes of ZrO_2, 18.8 tonnes of Fe, 3.43 tonnes of Cr, 1.9 tonnes of Ni, 12.5 tonnes of Zr and about 400kg of fission product material.

Four calculations have been performed. These have been performed with the ablation temperature of the concrete set to 1420K or 1600K (the input solidus and liquidus temperatures for the concrete respectively), with CORCON2.04.TRANC or CORCON2.04.00. The results for thermal penetration vertically into the basemat are plotted in figure 5. This shows that the differences caused by using different ablation temperatures are far greater than the long term differences caused by using TRANC or the original code. The exception is that an instability occurs in the CORCON2.04.00 run with an ablation temperature of 1600K at about 2×10^5 seconds. This is caused by the concrete interface temperature dropping below 1600K which forces the heat into the concrete to be zero which leads to a temperature rise to above 1600K which then drops below 1600K and repeats the cycle. A small amount of concrete is ablated in each cycle leading to increased vertical penetration. This oscillation is expected to occur for all timesteps however small but for sufficiently small timesteps should not lead to significant ablation.

5. Discussion

TRANC allows the transient conduction of heat into the concrete basemat to be modelled. The importance of this process depends on the particular situation being modelled. In general, for plant calculations, there is expected to be a phase for which the simpler steady state ablation calculations are accurate. This is when the entire melt-concrete interface is ablating at nearly the steady state rate. The steady state ablation calculations may also be accurate if some or all of the boundary is not ablating provided that the heat fluxes in other directions are sufficiently large. The steady state ablation approximation is not expected to be accurate at early times. These times are of particular relevance to experiments and to calculation of aerosol formation and fission product release. However, there may also be non-quasi-steady-state phenomena in the melt which are not modelled by CORCON.

6. Future Work

The following areas are the most important ones where TRANC could be improved.

1) Gas Release

Gas release is a very important phenomena. The present model is probably accurate for steady state ablation but has no mechanistic basis for the transient conduction case. It may be necessary to use a coupled heat transfer and gas release model in which the heat conduction equation would be modified.

2) Two Dimensional Conduction

The conditions for the quasi 1-D model for conduction to be accurate are usually not strictly satisfied. The thermal penetration distances can exceed the length scales associated with the melt front. However 2-D effects are only expected to lead to smoothing of the melt boundary and to have little effect on the downward penetration. 2-D calculations should also model the concrete in the region above the level of the melt.

7. Acknowledgements

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Appendix 1 : Stability of Thermal Penetration Schemes.

Ablation Problem

The stability of the scheme is investigated assuming that the heat flux ϕ into the concrete is constant.

Explicit time discretisation

The explicit scheme (as used in INTERUK [2]) is

$$\frac{\delta^n - \delta^o}{\Delta t} = \frac{(n+1)}{\rho L}\left(k\,\frac{(L+c(T_m - T_\infty))}{\delta^o} - \phi\right)$$

This can be written

$$\delta^n = f(\delta^o) = \delta^o + \frac{A}{\delta^o} - B$$

where

$$A = \frac{\Delta t(n+1)}{\rho Lc}\,k\,(L+c(T_m-T_\infty))$$

$$B = \frac{\Delta t(n+1)\phi}{\rho L}$$

Now

$$f(\delta_1) - f(\delta_0) = \delta_1 - \delta_0 + A\left(\frac{1}{\delta_1} - \frac{1}{\delta_0}\right)$$

$$= (\delta_1 - \delta_0)\left(1 - \frac{A}{\delta_1\delta_0}\right)$$

therefore

$$\left|f(\delta_1) - f(\delta_0)\right| < C\left|\delta_1 - \delta_0\right|$$

for $\delta_0, \delta_1 > \delta > 0$

where

$$C = \left|1 - \frac{A}{\delta^2}\right|$$

$$C < 1 \quad \text{if} \quad \delta^2 > \frac{A}{2}$$

Therefore, using the contraction mapping theorem, the scheme is stable provided

$$\delta^2 > \frac{A}{2}$$

i.e.

$$\Delta t < 2\delta^2 \frac{\rho c}{k} \cdot \frac{L}{(L+c(T_m - T_\infty))}$$

<u>Implicit time discretisation</u>

The implicit scheme is

$$(\delta^n)^2 + (a\Delta T - \delta^o)\delta^n - b\Delta t = 0$$

where $a = \dfrac{(n+1)}{\rho L} \phi > 0$

$$b = \frac{(n+1)}{\rho Lc} k(L+c(T_m - T_\infty)) > 0 .$$

This implies

$$\delta^n = \frac{\delta^o - a\Delta t \pm ((\delta^o - a\Delta t)^2 + 4b\Delta t)^{1/2}}{2}$$

As $\Delta t \to \infty$, $\delta^n \to \frac{b}{a}$ (steady state) and as $\Delta t \to 0$, $\delta^n \to \delta^o$, therefore take + sign:

$$\delta^n = f(\delta^o) = \frac{\delta^o - a\Delta t + ((\delta^o - a\Delta t)^2 + 4b\Delta t)^{1/2}}{2}$$

Now

$$f(\delta_1) - f(\delta_0)$$

$$= \frac{1}{2}\,(\delta_1 - \delta_0 + ((\delta_1 - a\Delta t)^2 + 4b\Delta t)^{1/2} - ((\delta_0 - a\Delta t)^2 + 4b\Delta t)^{1/2})$$

$$= \frac{1}{2}\,(\delta_1 - \delta_0)(1 + \frac{\delta_1 + \delta_0 - 2a\Delta t}{((\delta_1 - a\Delta t)^2 + 4b\Delta t)^{1/2} + ((\delta_0 - a\Delta t)^2 + 4b\Delta t)^{1/2}})$$

But

$$(\delta - a\Delta t)^2 \leqslant (\delta - a\Delta t)^2 + 4b\Delta t$$

which implies:

$$\left| \delta - a\Delta t \right| \leqslant ((\delta - a\Delta t)^2 + 4b\Delta t)^{1/2}$$

$$\Rightarrow \quad \left| \delta_1 - a\Delta t \right| + \left| \delta_0 - a\Delta t \right| \leqslant ((\delta_1 - a\Delta t)^2 + 4b\Delta t)^{1/2}$$

$$+ ((\delta_0 - a\Delta t)^2 + 4b\Delta t)^{1/2}$$

$$\Rightarrow \quad \frac{\left| \delta_1 - a\Delta t + \delta_0 - a\Delta t \right|}{((\delta_1 - a\Delta t)_2 + 4b\Delta t)^{1/2} + ((\delta_0 - a\Delta t)^2 \; 4b\Delta t)^{1/2}} \leqslant 1$$

(triangle inequality)

Therefore f is a contraction mapping and the scheme is stable for all $\Delta t>0$.

Appendix 2: Accuracy of Thermal Penetration Scheme for Fixed Boundary Problem

Consider the problem:

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} \qquad x>0, \ t>0$$

$$\left. \frac{-\partial T}{\partial x} \right|_{x=0} = \phi(t) \qquad t>0$$

$$T = 0 \quad \text{at} \quad t = 0, \ x \geq 0$$

$$T \rightarrow 0 \quad \text{as} \quad x \rightarrow \infty \quad \text{for} \quad t > 0$$

Let $\phi(t)$ be piecewise constant

$$\phi(t) = \phi_i, \ t_{i-1} < t \leq t_i \qquad i=1,2 \ \ldots..$$

$$(t_0 = 0, \ \phi_0 = 0)$$

The exact solution is

$$T(x,t) = \sum_{\{i:t_i < t\}} (\phi_{i+1} - \phi_i) \ f\ (x,t-t_i)$$

where

$$f(x,t) = 2 \left(\frac{t}{\pi} \right)^{1/2} \exp \left(\frac{-x^2}{4t} \right) - x \ \mathrm{erfc} \left(\frac{x}{2\ (t)^{1/2}} \right)$$

This can be rewritten as

$$T(x,t) = \sum_{1 \leq i \leq m-1} \phi_i (f(x,\ t-t_{i-1}) - f(x,\ t-t_i)) + \phi_m \ f\ (x,\ t-t_{m-1})$$

where

$$t_{n-1} < t < t_n$$

=>

$$T(0,t) = \sum_{1 \leqslant i \leqslant m-1} \phi_i \left(2\left(\frac{t-t_{i-1}}{\pi}\right)^{1/2} - 2\left(\frac{t-t_i}{\pi}\right)^{1/2}\right)$$

$$+ \phi_m\, 2\left(\frac{t-t}{\pi}\right)^{1/2}$$

where $t_{m-1} < t < t_m$

The thermal penetration solution is

$$T_w(t) = \frac{\phi_{i+1}}{k} \left(2\frac{k}{\rho c}(t-t_i)\frac{(n+1)}{(n+2)} + (\delta_i^+)^2\right)^{1/2}$$

The sum in the exact solution tends to zero as $t \to \infty$ therefore

$$\left| T_w(t) - T(0, t) \right| \to 0 \quad \text{as} \quad t \to \infty$$

for $\dfrac{n+1}{n+2} = \dfrac{2}{\pi}$ i.e $n = \dfrac{4 - \pi}{\pi - 2} = 0.7159 \ldots$

However, the heat content is incorrect. If $n=0$ the heat content is correct, but then T_w is incorrect as $t \to \infty$.

The thermal penetration scheme goes wrong if ϕ changes sign.

A test problem is shown in figure 6 which allows the accuracy of the scheme to be assessed. The approximate solution has a discontinuity in the value of T at $x=0$ when the exact solution has infinite values of $\left.\frac{\partial T}{\partial t}\right|_{x=0}$.

Appendix 3: Changed Format for Data Set.

IGEOM in columns 11-15 of record 2 of the data set is used to control whether the transient conduction models of TRANC are used. If IGEOM is less than 10 then the original CORCON MOD2 model is used. If IGEOM is greater than 9 then the new models are used and 10 is subtracted from IGEOM which then has the usual meaning.

If TRANC models are selected another input group is inserted after Group 10 (called Group 10a)

Group #	Field	Format	Variable Name
10a	1-10	E10.0	WN
	11-20	E10.0	TCOND
	21-30	E10.0	DELØ
	31-40	E10.0	TIMFAC
	41-50	E10.0	ER
	51-60	E10.0	TCO2

Appendix 4 : New COMMON Blocks Added in TRANC

None of the existing COMMON blocks in CORCON MOD2 have been changed. The following COMMON blocks have been added:

/ARGE/	contained in	FILM, INTEMP, MASRAT
/CNTRL/	contained in	CONPRP, CORCON, DATAIN, EDIT, FIXD, MOVD, QWALL, RECEDE, SURFEB, TIMSTP
/PHYS/	contained in	CONPRP, FIXD, MASRAT, MOVD, QWALL, SURFEB, TIMSTP
/STORE/	contained in	CONPRP, EDIT, INTEMP, MASRAT, MHTRAN, QWALL, RECEDE, TIMSTP

Principal Variables

The following principal variables are added in the new common blocks. For the arrays the index I represents a species, J a body point and L a layer.

CPCON	-	SPECIFIC HEAT OF CONCRETE
DELØ	-	INITIAL THERMAL PENETRATION DISTANCE
DELN	-	THERMAL PENETRATION IN CONCRETE
DELTA(J)	-	THERMAL PENETRATION IN CONCRETE AT OLD TIME
DELTAN(J)	-	THERMAL PENETRATION IN CONCRETE AT NEW TIME
ER	-	ENHANCEMENT PARARMETER FOR GAS RELEASE
GENRAT(J)	-	GAS GENERATION RATE
GMD	-	GAS GENERATION RATE
HFILM	-	SPECIFIC ENTHALPY OF GAS
HFLM(J)	-	SPECIFIC ENTHALPY OF GAS IN FILM
HLAT	-	LATENT HEAT OF MELTING OF CONCRETE
ICOND	-	FLAG TO INDICATE CONCRETE CONDUCTION MODEL
QIN	-	INTEGRAL OF HEAT FLUX TO CONCRETE
QMD	-	HEAT FLUX TO CONCRETE
QMDA(J)	-	HEAT FLUX INTO CONCRETE
SAGAS(I,J)	-	MASS RATE FRACTION OF GAS SPECIES RELEASED FROM CONCRETE
SFG(I,L)	-	MASS RATE OF EACH GAS SPECIES GOING INTO LAYER

SFGL(I,L)	-	MASS RATE OF EACH GAS SPECIES GOING INTO FILM
SGAS(I)	-	MASS FRACTION OF SPECIES OF GAS RELEASED FROM CONCRETE
SWFILM(I)	-	INTEGRAL OF SPECIES MASS ADDITION RATE OF GAS GOING TO FILM
SWGIN(I)	-	INTEGRAL OF SPECIES MASS ADDITION RATE OF GAS GOING TO MELT
TCO2	-	CO2 RELEASE TEMPERATURE
TCOND	-	THERMAL CONDUCTIVITY OF CONCRETE
TEDITN	-	TIME FOR NEXT BUT ONE OUTPUT
TIC	-	INITIAL TEMPERATURE OF CONCRETE
TIMFAC	-	TIME STEP CONTROL PARAMETER
TWA	-	CONCRETE/FILM INTERFACE TEMPERATURE
TWALL(J)	-	CONCRETE/FILM INTERFACE TEMPERATURE AT OLD TIME
TWALLN(J)	-	CONCRETE/FILM INTERFACE TEMPERATURE AT NEW TIME
TWL(L)	-	TYPICAL TEMPERATURE OF CONCRETE/FILM INTERFACE IN LAYER
WHFILM	-	INTEGRAL OF ENTHALPY ADDITION RATE OF GAS GOING TO FILM
WHGIN	-	INTEGRAL OF ENTHALPY ADDITION RATE OF GAS GOING TO MELT POOL
WN	-	PARAMETER FOR THERMAL PENETRATION WEIGHTING FUNCTION

Appendix 5 :

Routine by Routine Description of New or Changed subroutines

ANGAVL*

An additional test has been included to prevent an illegal call to ATAN2 with arguments (0.0,0.0).

CONPRP

In addition to the usual calculations this routine reads in WN, TCOND, TELO, TIMFAC, ER and TCO2 from the data file. It initialises HFLM(J), GENRAT(J), QMDA(J), TWALL(J), DELTA(J) and SAGAS(I,J). It also calculates HLAT and CPCON. The parameters are written to the output file.

CORCON

TEDITN is initialized and the call to TIMSTP has been moved earlier in the calling sequence so that the timestep is available when INTEMP and MASRAT are called.

DATAIN

This routine detects whether the new models in TRANC have been selected. If IGEOM is greater than or equal to 10, ICOND is set equal to 1 to indicate TRANC has been selected and IGEOM is reduced by 10.

EDIT

Additional output of DELTAN(J), TWALLN(J) and GENRAT(J) is provided. TWALLN(J) is used to calculate heat fluxes across the film instead of using TW or setting the heat flux to zero. TEDITN - the time of the next but one call to EDIT is now calculated.

FILM

There have been major changes to FILM. Additional arguments passed to FILM are DLT1, TWAL1, DLT2 and TWAL2 which are the thermal penetration distances and film/concrete interface temperatures at positions 1 and 2 at the old time. Other new arguments are passed in common /ARGE/. The gas generation rate (GMD) is now varied in the iteration instead of the ablation rate (EMD). If the original simple iteration fails a robust solver is called. This is based on the NAG [6] routines CØ5AVF and CØ5AZF. There is scope for improving the speed of this routine.

FIXD

FIXD is a new routine. It calculates the new thermal penetration distance and film/concrete interface temperature when the concrete is not melting.

FQWALL

FQWALL is a new function called by QWALL. It calculates the heat flux across the gas film for a specified melt pool/film interface temperature, heat transfer coefficient and heat flux into the concrete.

HTRLAY*

A FORMAT statement has been corrected.

INTEMP*

Various changes have been made to allow the ablation rate, gas generation rates of each species, heat flux and enthalpy of gas to be non proportional. A duplicate data definition has been removed.

MASSEX*

A duplicate data definition has been deleted.

MASRAT

Various changes have been made to allow for the ablation rate, gas generation rates, heat flux and gas enthalpies to be non-proportional. The concrete/film interface temperature is also allowed to change.

MHTRAN

Changes have been made to allow the concrete/film interface temperature to vary. The composition of the gas from the concrete is also allowed to vary.

MOVD

MOVD is a new routine. It calculates the new thermal penetration distance and ablation rate when the concrete is ablating.

QMELT

A bail-out has been added. If QMELT would have calculated a heat flux from the concrete into the pool then the heat flux is set to zero. This should only occur in early iterations or in exceptional conditions.

QWALL

QWALL is a new routine. For a given pool/film interface temperature it calculates the new thermal penetration distance, concrete/film interface temperature and ablation rate such that the heat flux across the film balances the heat flux into the concrete. The NAG [6] routines CØ5AVF and CØ5AZF are used.

RECEDE

This routine now also interpolates the film/concrete interface temperatures and thermal penetration distances on to fixed rays.

SURFEB

SURFEB has been largely rewritten to use NAG [6] routines CØ5AVF and CØ5AZF instead of the Newton solver. It now calls QWALL as an analogue to calling QMELT.

TIMSTP*

TIMSTP has one bug fix which includes the modification for internal corners that was added to RECEDE in CORCON MOD2. It also can impose an addition constraint on the timestep based on the peclet number associated with conduction in the concrete.

* Denotes that corrections have been made to these routines which should be included in the original CORCON2.04.00. They are identified by CULFX in the modification set.

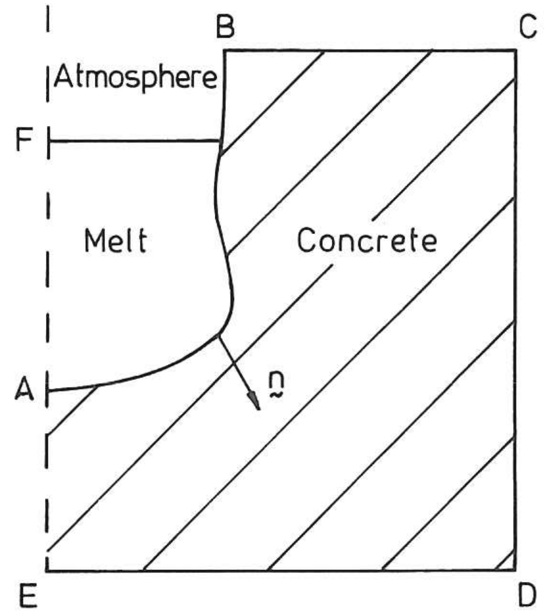

Fig. 1 Melt concrete configuration

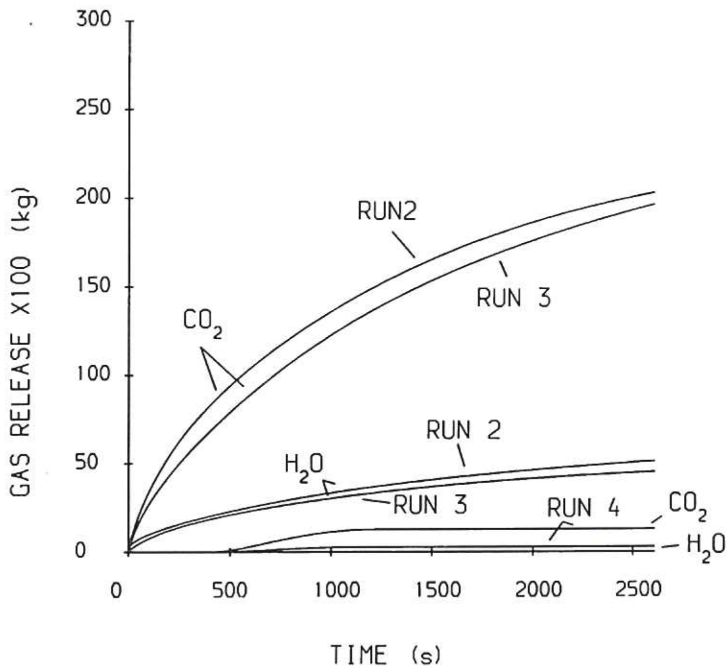

Fig. 2 Calculated cumulative releases of gases for TURC-2. (Refer to table 1 and text for further details)

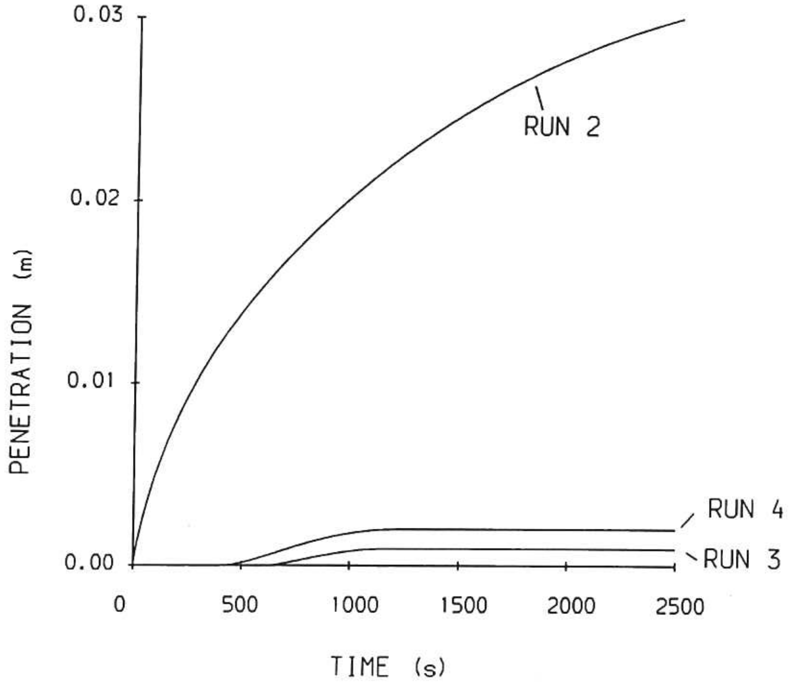

Fig. 3 Calculated vertical melt penetration for TURC-2. (Refer to table 1 and text for further details).

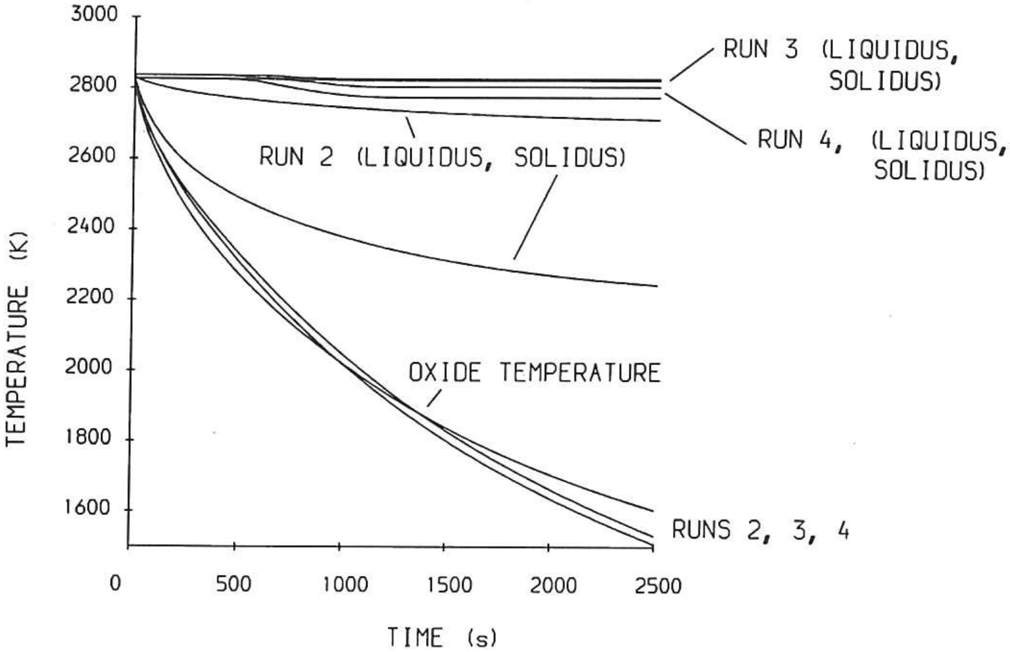

Fig. 4 Calculated liquidus, solidus and average temperature for TURC-2. (Refer to table 1 and text for further details.)

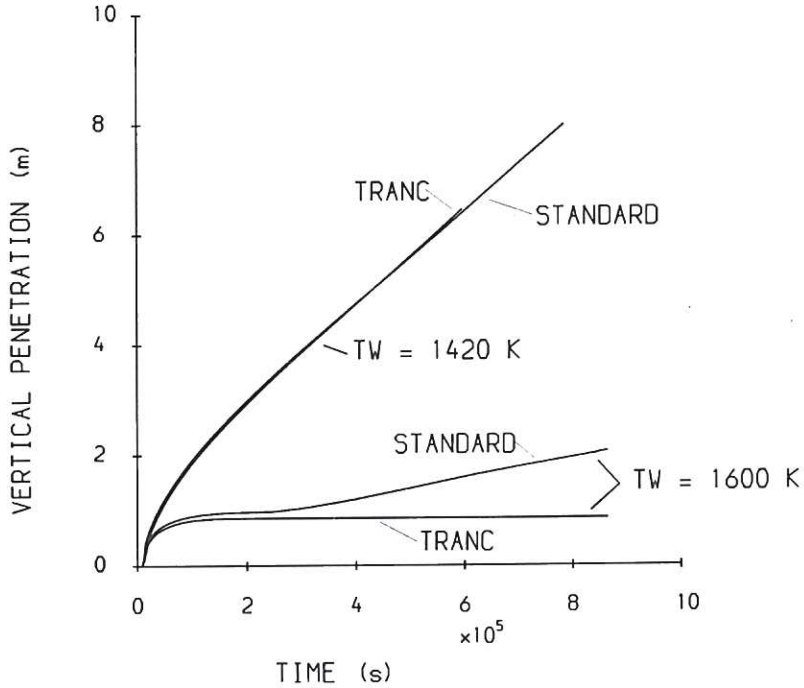

Fig. 5 Vertical melt penetration for plant calculations. The cases shown are for a concrete ablation temperature of 1600K (the liquidus) or 1400K (the solidus) and with or without the TRANC modifications for heat transfer in the basemat.

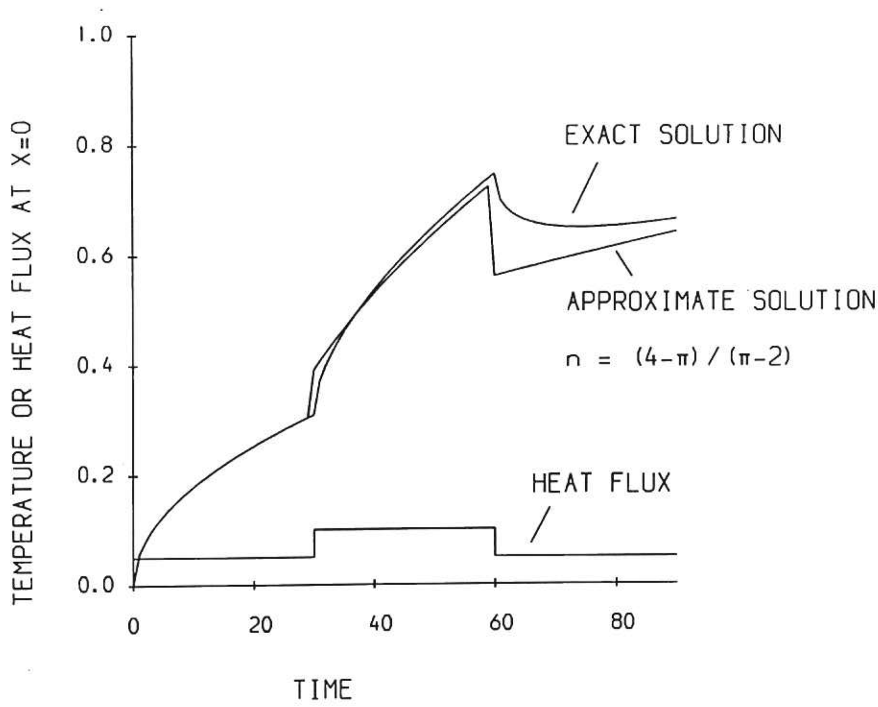

Fig. 6 Comparison between the exact solution and the thermal penetration approximation to a 1-D thermal conduction problem.

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