Modelling heat transfer and dissolved species concentrations within PWR crud

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The crud formed on PWR fuel tends to contain "chimneys" penetrating down to the metal surface. This provides an opportunity for wick-boiling to occur. This is associated with the generation of very high concentrations (many tens of times the bulk values) of dissolved species within the crud, and associated significant increase in the local saturation temperature. These both have consequences for cladding corrosion, and the accumulation of boron in the crud contributes to the phenomenon termed "axial offset anomaly". We present here detailed, coupled two-dimensional models of these processes, which allow the three linked phenomena, heat conduction, advection and diffusion of species in the water, and diffusion of the water itself, to be modeled and their aggregate effect to be seen.

1 INTRODUCTION

Crud formation in water-cooled reactors has caused operational problems from the beginning of nuclear power, and continues to do so. Crud layers are chemically very complex, resulting from the deposition of various species present within the coolant. Some, like boron, are added deliberately, and others are present essentially as corrosion products from other parts of the coolant circuit. They cause a variety of problems, including increased cladding corrosion, by either increased cladding temperatures or changed chemical conditions, or some combination thereof, and power distortions and reductions due to the undesirable accretion of boron onto the surface of the cladding[1, 2].

In this paper we develop a two-dimensional, coupled, model of some of the main phenomena thought to contribute to these effects, with the aim of predicting cladding temperatures and concentrations of dissolved material in the coolant in the pores of the crud.

In Section 2 we describe the background to the crud problem in more detail, mentioning some of the main earlier work upon which the present analysis builds. In Section 3 we describe the physical basis of our coupled model, of the heat conduction, the flow of water to hot regions where wick boiling is occurring, and the associated advection and diffusion of the dissolved species, and the way in which these three effects are all mutually coupled. In Section 4 we describe the numerical implementation of this coupled model, via a finite volume scheme. In Section 5 we present results from the application of the model, investigating the significance of the coupling, and draw conclusions in Section 6.

2 BACKGROUND

In a water-cooled reactor, very hot water flows over large areas metal, and consequently metallic ion species become dissolved within it. In addition, in PWR reactors, it is common to add boric acid into the coolant for reactivity control.

Several of these dissolved species precipitate on hot fuel pin surfaces within the reactor, in particular because for many of them solubility decreases with increasing coolant temperature. In addition, these deposits can contain insoluble materials, such as chromium and zirconium species, transported in particulate form by the coolant. These deposits, commonly termed "crud", have various effects upon the reactor. Principal amongst them are that coating of the surfaces of the fuel pins changes the thermal-hydraulic conditions and cladding temperature, and that higher concentrations of dissolved species within the crud can accelerate cladding corrosion. Another consequence that has received particular attention of late is known as "Axial Offset Anomaly", AOA. This relates to the fact that the crud provides a mechanism for the concentration of boron from the coolant. Because of the inverse solubility mentioned

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above, this predominantly occurs in the upper half of the core. The increased boron concentration reduces the neutron flux, and hence the power output, in the upper part of an affected core. This skewed axial power distribution has given rise to the term AOA[1-4].

The solid formed typically has a porosity of about 60-80% (although there is some inevitable uncertainty as to just how closely *a posteriori* measured values mirror in-reactor conditions)[5]. In addition, there are generally channels ("chimneys") from the crud surface through its thickness down to the surface of the cladding. One consequence of this structure is that it permits a mechanism termed *wick boiling*, where liquid soaks through the porous crud until it reaches a region where the temperature is above the local saturation temperature, and there is a channel available for the egress of the vapour produced[6, 7].

All of these phenomena have been studied in some detail over many years.

In 1971 Macbeth[7] developed a one-dimensional hydraulic model of flow in a chimney-filled crud, and studied the effect of chimney population density, although this model was not able to determine temperature distributions or solute concentrations.

In 1974 Cohen[5] developed a one-dimensional model for heat and mass transfer through a porous crud layer, along the lines of heat transfer along a fin. Heat was modeled as being conducted away from the cladding, and lost laterally via evaporation into the chimney. An inwards mass flow rate of water, sufficient to replace this evaporative loss, was then computed. From this, *inter alia*, an estimate of the temperature beneath the crud was obtained[5].

In 1985 Pan[8] presented a two-dimensional analysis of the mechanism, computing the temperature distribution as a function of depth into the crud, and of the radial distance from the chimney. In 1987 he presented[9] an further analysis of chimney-populated crud, under wick boiling conditions. In this he computed the concentrations of the various dissolved species that were reached. Whilst these analyses incorporated two-dimensional effects, they are not able to allow for the various interactions between the phenomena at work. A parameter survey was performed, giving some insight into the dependence on, for example, crud thickness, porosity and chimney density. The model indicated that dissolved species concentrations increased with crud thickness, with decreasing porosity, and with increasing chimney population.

More recently, significant strides have been made in understanding of the physical chemistry of the crud, and its coupling to the associated thermal conditions, by Henshaw and colleagues[10], building upon the Cohen work. They developed a one-dimensional (through-thickness) model that couples thermal hydraulics with the water chemistry. Postulating heat transfer through wick boiling, they modeled to the downward flow of water soaking through the crud, evaporating into steam at the surface of the chimneys. A particular advance of the model was to investigate the various chemical reactions taking place within the porous deposits. These reactions are generally temperature dependent, and a degree of coupling between the reaction rates, and the temperatures caused to obtain by the species thus caused to be present, was incorporated.

In this present work we have developed a more representative two-dimensional model, that couples mechanistically the processes which are in principle present; heat transfer through the wet crud, diffusive flow and boiling of the water at chimney surfaces to remove the heat, and the advection and diffusion of dissolved species. Our model also provides a framework within which the further, more sophisticated, physical chemistry analysis of Henshaw and colleagues can in due course be incorporated.

3   THE PHYSICAL BASIS OF THE MODEL

3.1   INTRODUCTION

As noted above, in addition to the usual convective heat transfer from the surface of the crud, the presence of the deep, slender chimneys offers the possibility of the additional heat transfer mechanism of evaporation from the surface of the chimney. The passage of heat through the crud will be by conduction through the crud itself, and through the water in the

pores of the crud. Evaporation from the surface of the crud into the chimney will require a flow of water through the crud to the chimney face.

The flow of the water will take the form of the usual flow through a porous medium, drawn by the evaporative mass flux at a chimney surface, entering the crud at the face exposed to the bulk coolant, and leaving in the form of vapour formed at the walls of the chimneys.

The liquid coolant that enters the crud in this fashion will of course contain within it whatever species are present in solution in the coolant. As discussed above, these include in particular boric acid. At the chimney surface, the evaporation will lead to the removal only of steam, and thus water flowing into the crud cannot (in the steady state) carry into the crud those species dissolved within it. What must happen is that a spatial variation of the concentration of the dissolved species will be generated, with an increase in this concentration in going from the wetted surface of the crud to the chimney. The dissolved species will diffuse down this concentration gradient (ie away from the chimney surface), canceling out the advection of the dissolved species associated with the flow of the water. Everywhere, but in particular at the chimney surface, the concentration of dissolved species will be higher than in the bulk coolant. This will have various consequences, but that of most immediate interest is that the increased concentration of dissolved species may affect the saturation temperature of the coolant, changing the thermal conditions at the chimney face.

As will be seen, these three processes are all linked. The rate of heat transfer by evaporation at the chimney wall plainly depends upon the saturation temperature there. The saturation temperature depends on the concentration of dissolved species there. The concentration depends on the advective flow, and this flow is determined by the rate of heat transfer by evaporation at the chimney wall.

In the sections that follow we will expand upon these issues, identifying the associated governing equations that describe them, and the relevant boundary conditions.

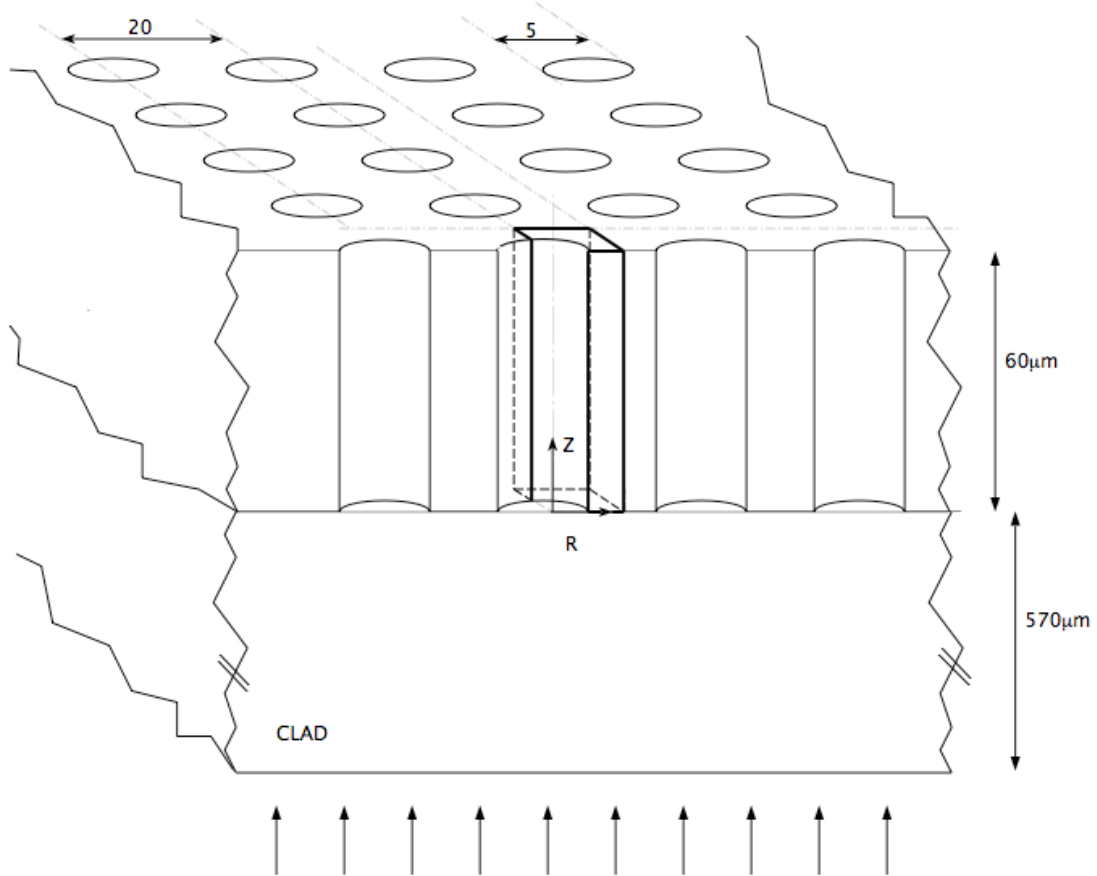A schematic depiction of a chimney-filled crud, and the region analysed, is shown in Figure 1.

Figure 1
A schematic diagram, showing the crud, chimneys and clad, with characteristic dimensions in microns. The region analysed in our model is indicated, along with the coordinate system used to identify the results we present.

3.2 HEAT CONDUCTION

We model the heat transfer through the wetted crud via Laplace's equation:

$$\nabla^2 T = 0 \qquad (1)$$

(There is in addition advection of heat because of the flow of the water, but this is negligible; the water flow rate is tiny.) Boundary conditions are adiabatic on planes of symmetry bounding the region modelled, an imposed uniform heat flux on the inner face of the crud, and an imposed (saturation) temperature on the face of the chimney:

$$T\left(\mathbf{r} \in \text{CHIMNEY SURFACE}\right) = T_{\text{SAT}}\left(\mathbf{r} \in \text{CHIMNEY SURFACE}\right) \qquad (2)$$

(One could instead employ Robin boundary conditions, with a (very high) evaporation heat transfer coefficient; the approach above effectively takes this heat transfer coefficient to be infinite. The results from both approaches are essentially identical.) The value of the saturation temperature depends on the concentration of the dissolved species. The concentrations are found from solution of Equation (9) below. The main species to affect the saturation temperature, and the only one considered at present, is boron in the form of boric acid, (H_3BO_3). The dependence of saturation temperature on boron concentration is taken from the correlation published by Deshon[4], applicable at PWR conditions, and is shown in Figure 2.

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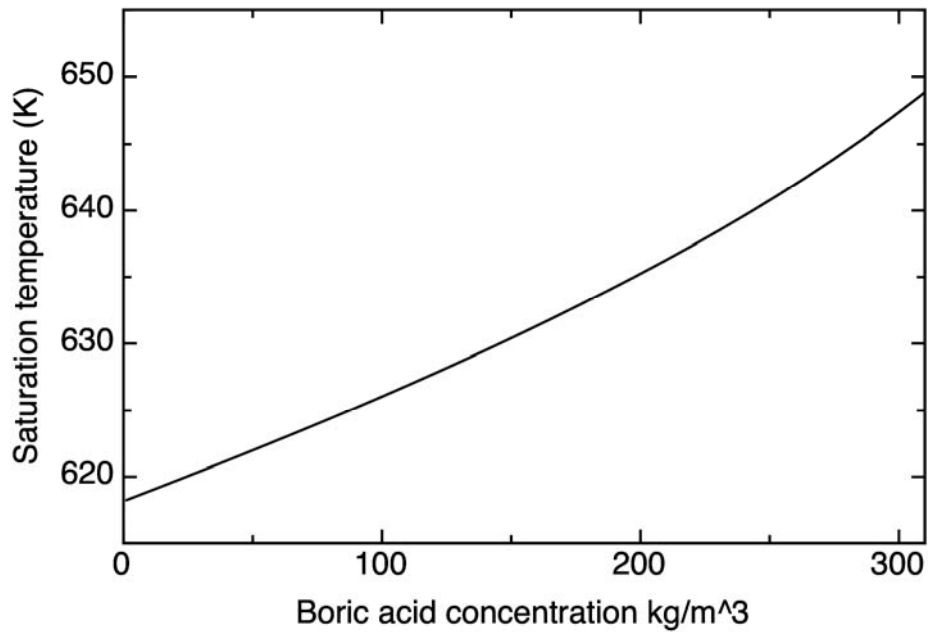Figure 2
The dependence on boron concentration of the saturation temperature of water at 15.55 MPa, taken from the correlation published by Deshon[4].

Interaction with the bulk coolant flow is via a specified heat transfer coefficient and bulk coolant temperature. These boundary conditions are indicated in Figure 3.
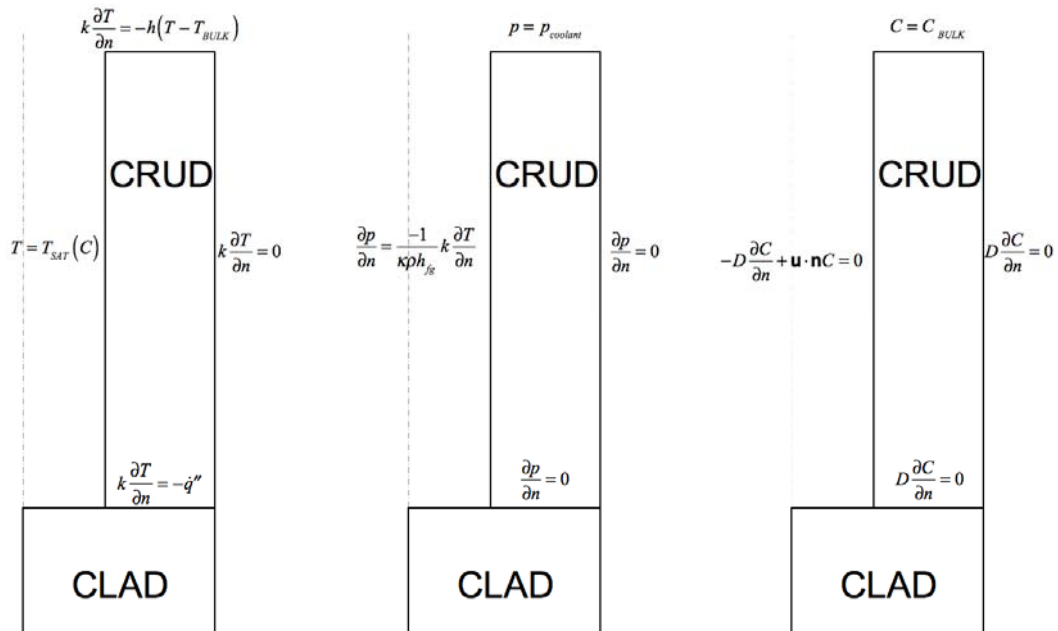

Figure 3
Boundary conditions for (from left to right) the temperature, flow and concentration analysis. The dashed lines are the chimney axes, and the right hand boundaries represent the plane of symmetry assumed as a consequence of the neighbouring chimney.

3.3 THE DIFFUSIVE FLOW OF THE COOLANT THROUGH THE CRUD

The flow of water through the crud is modeled as a diffusive flow, with the local velocity related to the local pressure gradient via a flow resistance:

$$\mathbf{u} = -\kappa\nabla p \tag{3}$$

This results in a Laplace equation for the pressure distribution within the crud.

$$\nabla^2 p = 0 \tag{4}$$

Boundary conditions of no flow on planes of symmetry, and at the clad-crud interface, are employed.

At the chimney surface a spatially varying mass flow rate is imposed, based on the local heat loss rate:

$$\dot{m}h_{fg} = k\frac{\partial T}{\partial n} \tag{5}$$

This gives, in terms of the diffusive flow problem,

$$\frac{\partial p}{\partial n} = \frac{-1}{\kappa\rho h_{fg}}k\frac{\partial T}{\partial n} \tag{6}$$

These boundary conditions are indicated in Figure 3. The numerical value of $\dfrac{\partial T}{\partial n}$ for use in Equation (6) is found from the solution of Equation (1) above.

3.4 THE ADVECTION AND DIFFUSION OF THE DISSOLVED SPECIES IN THE CRUD

Denoting the concentration of dissolved species C, and their net flow (current) $\mathbf{J}$, we can write the net flow of dissolved species as the sum of advective and diffusive terms:

$$\mathbf{J} = -D\nabla C + \mathbf{u}C \tag{7}$$

In the steady state we have

$$\nabla \cdot \mathbf{J} = 0 \tag{8}$$

or, as $\nabla \cdot \mathbf{u} = 0$,

$$-D\nabla^2 C + \mathbf{u} \cdot \nabla C = 0 \tag{9}$$

The boundary condition at the crud-coolant interface is that the concentration is equal to the bulk coolant concentration. At the planes of symmetry and the clad surface the normal gradient of concentration is zero. The boundary condition at the chimney surface is that there is no net flow of dissolved species to the surface:

$$-D\frac{\partial C}{\partial n} + \mathbf{u} \cdot \mathbf{n}C = 0 \tag{10}$$

These boundary conditions are indicated in Figure 3. The required variation of the water velocity throughout the solution domain is provided by the solution of Equation (4), coupled with Equation (3). The boundary value of $\mathbf{u} \cdot \mathbf{n}$, or equivalently $\kappa\dfrac{\partial p}{\partial n}$, needed in Equation (10), is found from solution of (4) above.

3.5 THE COUPLED SOLUTION

There are three equations to be solved; the temperature distribution in the crud, the water velocity in the crud, and the distribution of the concentration of dissolved species in the crud. Each equation has boundary condition values that depend upon the solution of one of the

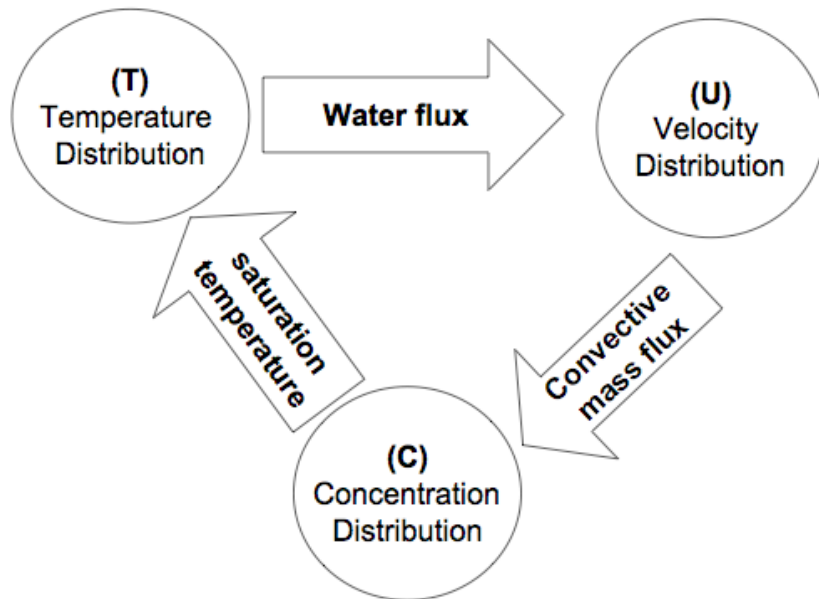other equations, and an iterative approach is taken to solve them. This is shown graphically in Figure 4.

Figure 4
The sequential, iterative solution of the three coupled equations, of temperature distribution, water flow and species concentration in the crud

4   NUMERICAL IMPLEMENTATION

In Figure 1 is indicated (one quarter of) the crud notionally associated with a single chimney. (Of course, real chimneys do not display the uniformity of diameter, or regularity of position, of that figure). We model the three-dimensional region shown as two-dimensional (R-z), approximating the two symmetry planes remote from the chimney by a circular arc, centred on the chimney.

The three equations to be solved, (1), (4), and (9), are solved numerically using a finite-volume scheme. The numerical approach is fairly standard, and we will not give any details here; a good introduction to the methods is provided by Versteeg[11]. The Peclet number is well below unity, so a central differencing scheme is used.

Equations (1) and (4) are in effect subsets of Equation (9); they both lack the advective term but are otherwise identical. From a practical point of view, this allows some economy in code development, as the code that solves the advection - diffusion equation can be employed with minimal modification to deal with the wholly diffusive equations.

For each of the three equations, once the boundary conditions are incorporated the finite volume discretisation generates a sparse matrix equation. This is solved using a standard 'line by line' iterative solver.

In this case, of course, the equations are coupled. Boundary conditions for any one equation are available only from a solution of the other two. We accommodate this by following the procedure implicit in Figure 4. Equation (1) is first solved for the temperature distribution, using the physical properties of water at a nominal coolant conditions. This solution is used to determine the flow-field in the crud, Equation (4). This flow field is then used to determine the concentration of the dissolved species. This concentration is then used to provide a modified saturation-temperature boundary condition for the temperature solution. This sequential solution of the three equations is of course automated. In practice, we find that the convergence of this iteration is smooth and quite rapid, with converged results being achieved in typically 5-10 iterations.

5   APPLICATION OF THE MODEL

5.1   INTRODUCTION

In the works cited earlier, Macbeth, Cohen and Pan studied variously one and two dimensional models of the crud, studying temperature, and later species concentration, with differing levels of sophistication. The more recent work Henshaw incorporated in a one-dimensional context coupling between species concentration and the local temperature.

In the first set of results presented here, we use the present coupled two-dimensional model, in a reduced form, to attempt to reproduce directly some of the earlier results of Pan. The intention of this is both to provide a degree validation, and to provide some indication of the changes in results occasion by the incorporation of the coupling into the model.

In the main body of our results we show predictions of temperature distribution and species concentration using the full coupled two-dimensional model.

For convenience, the values of the quantities used in the various analyses are listed in Table 1. Note that the limiting value of heat flux used, 1.5 MWm^{-2} at the clad/crud interface, corresponds to about 1.7 MWm^{-2} at the clad inner surface.

	Symbol	Units	Pan 1985	Pan 1987	Henshaw 2006	Present work
Crud thickness		μm	25	25	59	60[10]
Chimney centres		μm	15.96	20.6	20.6	20[10]
Chimney diameter		μm	5	5	5	5[10]
Crud porosity	ε	%	80	80	80	80[10]
Crud / water mean thermal conductivity	k	W m^{-1}K^{-1}	0.69	0.69	n/a	0.506[4]
Heat Flux	q	MWm^{-2}	1.11	1.80	1.11	1.5
System pressure	p	MPa	15.16	15.5	15.3	15.5
Boric acid diffusion coefficient	D	m^{2}s^{-1}	n/a	n/a	1.05E-08	1.05E-08
Li diffusion coefficient	D	m^{2}s^{-1}	n/a	1.7E-08	n/a	n/a
Tortuosity	Γ		n/a	0.4	0.4	0.4[10]
Coolant boron concentration	C_b	ppm (gm^{-3})	n/a	n/a	1200 (4637)	1200[10]
Coolant Li concentration	C_b	ppm (gm^{-3})	n/a	2 (1.4)	2	n/a
Coolant heat transfer coefficient	h	W m^{-2}K^{-1}	n/a	n/a	n/a	1.2E04[12]
Bulk coolant temperature	T	K	n/a	n/a	n/a	590

Table 1
The values of the parameters used in the various analyses.

5.2   VALIDATION AND ANALYSIS OF EARLIER MODELING

The earlier analysis of Pan[8] in 1985 computed for a two-dimensional model the radial and through-thickness variation of temperatures and water pressure in the vicinity of a crud chimney. Using the same data as Pan, and operating the present model in an uncoupled form, generates essentially identical results. Pan later extended his work[9] to address concentrations of dissolved species, and again with the same parameters employed, the

present model predicts the same results. Comparisons between Pan, and the use of the present model operated in an uncoupled form, are shown in Figure 5.
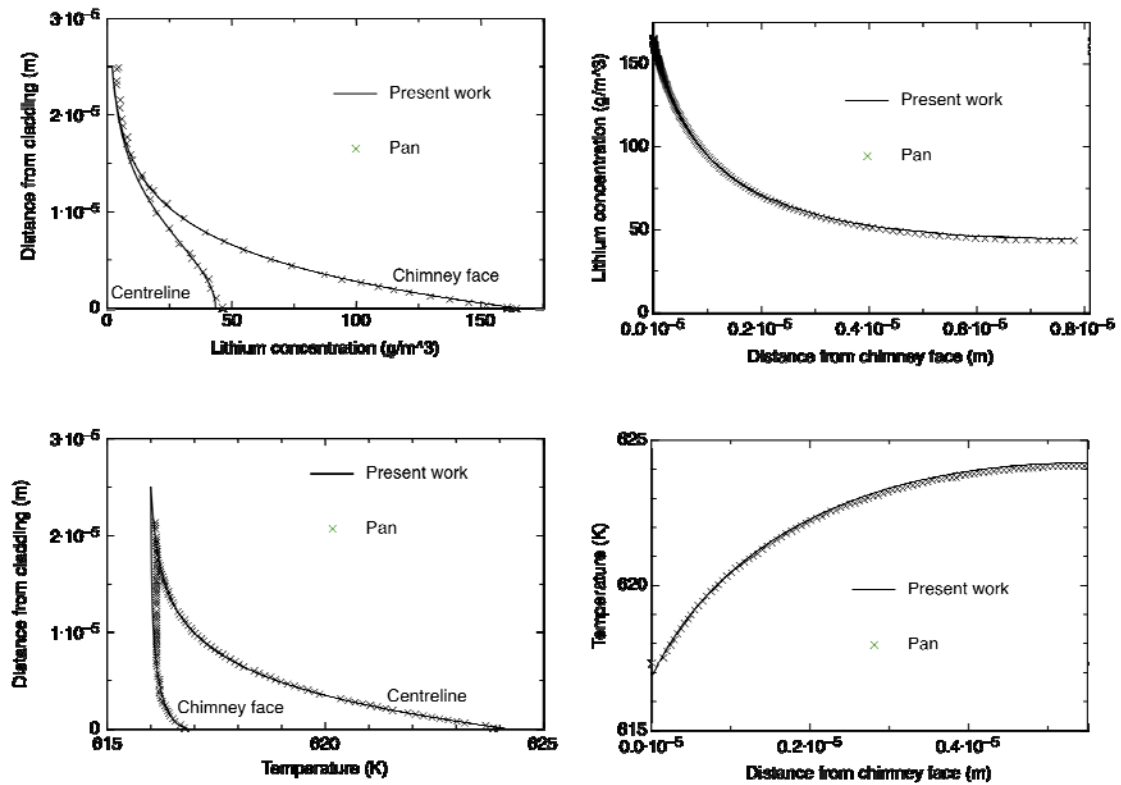

Figure 5
The use of the present model, in uncoupled form, to analyse the cases studied by Pan. (Radial variations are shown at only z=0; at the free surface values are prescribed as boundary conditions.)

5.3   TWO-DIMENSIONAL EFFECTS, AND THE COUPLING OF THE PHENOMENA

In the following two sections we apply the fully coupled two-dimensional model, using the parameter values from Table 1.

We here analyse the crud with the present two-dimensional model, with the coupling between the phenomena both incorporated and omitted. Results from this are shown in Figure 6. The concentration of the dissolved boric acid is seen to be ~25 times the bulk value at the inter-chimney centre line, but to rise by a further factor of two to ~55 times the bulk value at the chimney face.

For the purposes of the present analysis, the most important consequence of this is that the boiling point of the coolant at the chimney face is raised. Here the elevation is by about 25K, but naturally the actual numerical value depends on the parameter values adopted to characterize the crud and other conditions.
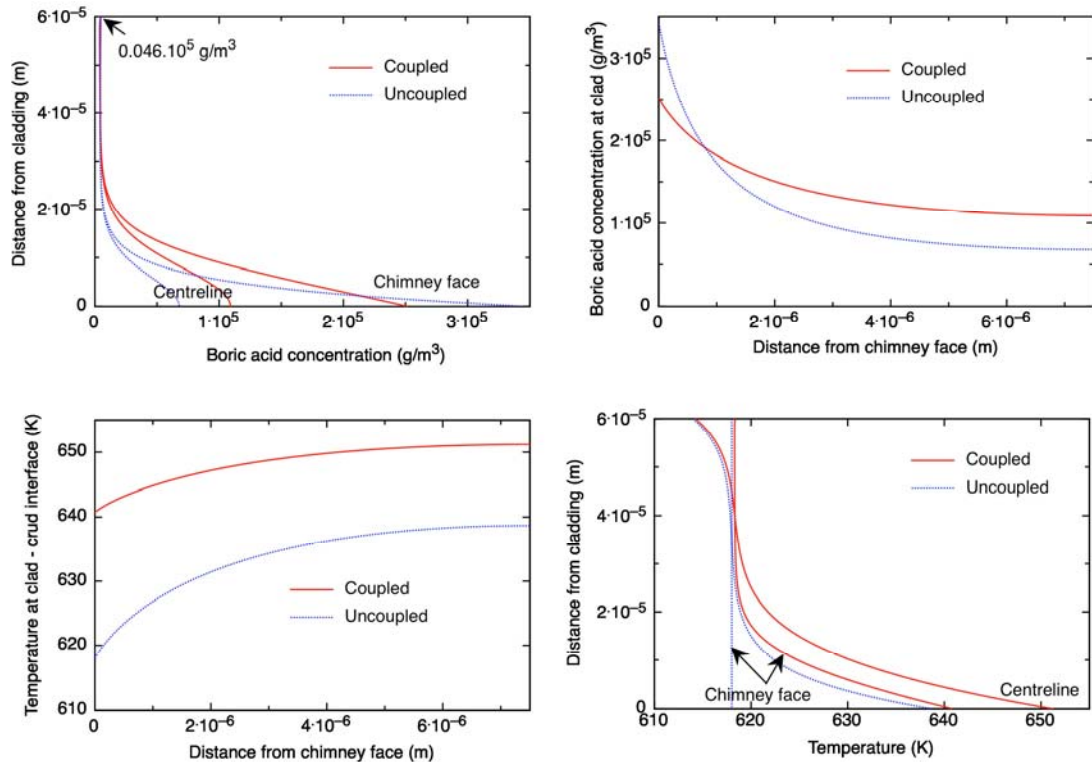
Figure 6
A comparison of models with the coupling between the three phenomena taken into account, and omitted. (As in Figure 5, radial variations are shown at only *z*=0; at the free surface values are prescribed as boundary conditions.)

5.4   HEAT TRANSFER MECHANISMS, AND THE ASSOCIATED FLOWS OF HEAT

The wick boiling addressed here is obviously an additional, different mechanism for heat transfer from the fuel to the coolant. We will investigate here its importance relative to the normal convective heat transfer to the liquid coolant.

For the (typical) geometry considered, the inside surfaces of the chimneys have an area approximately 3 times the area of the crud which is in contact with the liquid coolant. For the conditions studied, the heat flux from the wet crud surface to the coolant, if crud were not present, is 1.5 MWm^{-2}.

HEAT FLUX FROM CRUD
TO COOLANT CHANNEL
(PEAK VALUE ~0.3 MW/M^2)

COOLANT

CRUD

CRUD

Z

R   CLAD

HEAT FLUX FROM CRUD INTO
CHIMNEY
(PEAK VALUE ~3.5 MW/M^2)
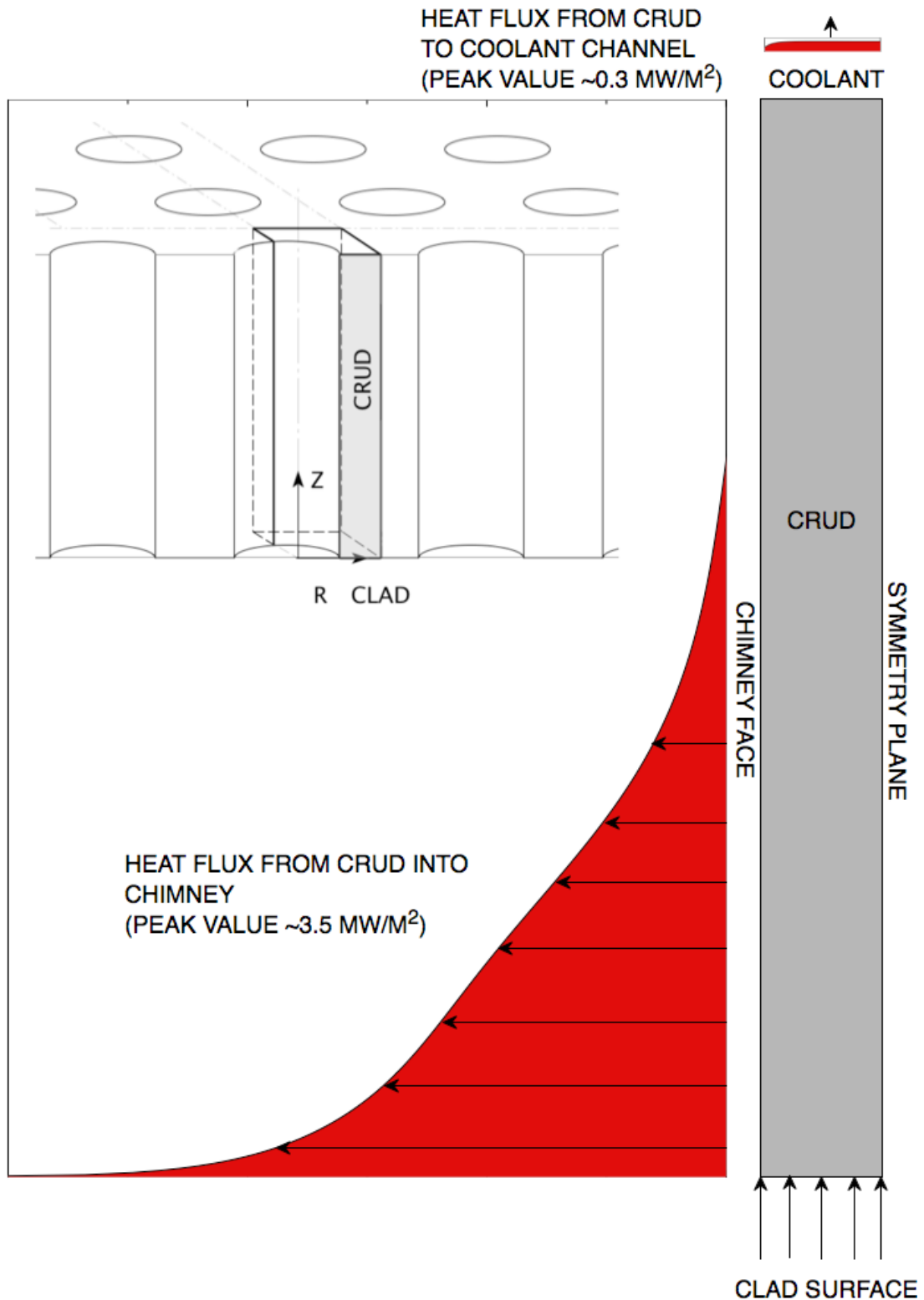
CHIMNEY FACE

SYMMETRY PLANE

CLAD SURFACE

Figure 7
The distribution of heat flux from the crud. The crud is indicated by the grey rectangle,
drawn to scale. The (large) graph to the left of the crud shows the heat flux into the chimney
surface by evaporation. The (small) upper graph shows the heat flux associated with normal
single-phase convection into the main coolant flow. The two graphs are drawn to the same
scale.

In Figure 7 we see that the heat flux is high into the chimney in regions close to the cladding, but that it falls rapidly. Wick boiling only occurs in the crud close to the clad. The convective heat flux to the coolant reduced to ~1/5 of its no-crud value.
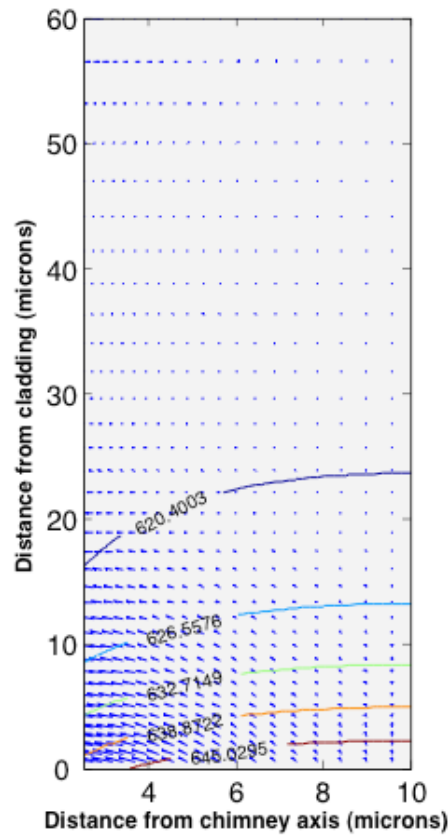

Figure 8

The 'cut face' of the crud from Figure 7, with the crud stretched in the radial direction for clarity. (The cladding thus lies below the horizontal axis, and the chimney is to the left of the vertical axis. On this cut face heat flow vectors are shown as arrowed straight lines. Also shown are curves indicating temperature contours.

In Figure 8 we show the flow of heat and temperature contours in the crud. Heat flow is seen to be overwhelmingly in the direction towards the face of the chimney, and to increase as the chimney is approached. It is notable that there is very little conduction of heat, in either direction, in other than perhaps the ~quarter of the crud closest to the clad. Similarly, temperature gradients and temperature was highest in this region, with very small temperature gradients in the outermost three-quarters of the crud.

Spatial integration of the heat fluxes over the chimney surface and over the wetted surface allows evaluation of the division of the total flow of heat between the two mechanisms to be determined. For the (typical) conditions considered here, some 80% of the heat is lost by evaporation into the chimney, and indeed into the lower one quarter of the chimney, with only 20% of the heat being taken away by single-phase convection at the wetted surface.

6   DISCUSSION AND CONCLUSIONS

The presence of "chimneys" in the crud coating the fuel permits a wick-boiling mechanism to take place. Coolant soaks into the crud, and evaporates at the chimney face. With no net flow of the dissolved species, high concentrations are established in the crud.

Physically consistent, coupled models have been developed of the processes of heat transfer, advection and diffusion of the dissolved species, and of the diffusion of water through the crud. Inter alia, these allow effects such as the dependence of saturation temperature on the

concentration of a solute to be taken into account. These confirm that high concentrations of dissolved species can be developed, with significant "radial" variations in concentration, alongside elevated temperatures.

This mechanism seems likely to be the dominant mode of the transfer of heat from the fuel to the coolant, accounting for perhaps 80% of the heat generated.

Further work planned with this model includes a parameter survey better to understand the range of the various parameters over which these effects are significant, and further development of the model to incorporate the additional physical chemistry effects proposed by Henshaw in his earlier one-dimensional treatment.

7   ACKNOWLEDGEMENTS

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