Chapter 8 - Technology of Accident Analysis

Introduction

The previous Chapter summarized the safety issues, accident by accident, for a CANDU. This chapter describes the underlying science of accident behaviour. As with other engineering disciplines, the objective of nuclear engineering is to operate the plant as economically as possible consistent with public and worker safety and environmental protection. Since nuclear plants are capital-intensive, and the fuel is cheap, this means that there is a strong incentive to extract the maximum power from a given plant. This leads to the usual tradeoff of large margins and simple analysis, versus smaller (but adequate) margins and sophisticated analysis; given the cost of a nuclear plant, the second route always wins out and drives an increasing sophistication in accident analysis tools and methodology. The same tradeoff and resolution is true of course of all other fields of engineering - e.g., aeroplane design.

In the early days of CANDU, for NPD and Douglas Point, the accident analysis was done by hand. Digital computers had barely made an impact on engineering, and as a result both performance and safety margins were (had to be) large, partly because of lack of experience and partly because of the simplifications which had to be made in order to do the calculations. The major areas of sub-optimization were in low fuel ratings, sub-cooled primary circuit conditions, low primary-side pressure etc. Nowadays almost **no** accidents are predicted using hand calculations - the physical models used in accidents have become far more detailed and are embedded in complex transient computer codes.

To list all these codes and consider them as black boxes is not very useful. So in this Chapter we shall describe the basic science underlying each safety-related discipline, and present in simplified form the types of models used. We borrow heavily from notes by D. Meneley, J.T. Rogers and W. Garland.

We shall not derive each model from first principles, having neither time nor space. The reader is referred to numerous textbooks for basic derivations. The purpose of the Chapter is therefore to highlight briefly the key physical models used in safety analysis so that the reader will recognize them in examining a topic in more depth.

Reactor Physics

We have already covered point kinetics in Chapter 3. Recall the basic kinetics equations:

$$\frac{dN_f(t)}{dt} = \frac{k_\infty(r - b)}{l_p} N_f(t) + \sum_{i=1}^{6} l_i C_i$$

and

$$\frac{dC_i}{dt} = \frac{b_i N_f(t)}{l_p(1 - r)} - l_i C_i$$

Unfortunately CANDUs cannot be considered point reactors. Strong spatial effects result from flux tilts (especially for large LOCA, if only half the core is voided - as in CANDU 6), insertion of shutoff rods from the top of the reactor, etc. Thus in practice one must use three dimensional diffusion equations in conjunction with the point kinetics[1]. The diffusion model tracks the neutrons as a flow through a medium, subject to scattering, absorption, and leakage. The basic diffusion equation is one of continuity. Consider a volume *V*. The time rate of change of neutrons within volume V must be equal to the rate at which they are produced within *V* minus the rate at which they are absorbed or escape from *V*. Thus if *n(**r**, t)* is the neutron density at (three-dimensional) point ***r*** and time *t*, then the continuity equation for *V* is

$$\frac{d}{dt}\int_V n(\mathbf{r},t)dV = production - absorption - leakage$$

Let *s(**r**,t)* be the number of neutrons emitted per unit volume per unit time by sources at the point ***r*** and time *t*. This is the *source distribution function*. Thus

$$production = \int_V s(\mathbf{r},t)dV$$

Likewise the absorption rate is the product of the flux *ö(**r**,t)* and the absorption cross section Ó$_a$(***r***) integrated over V:

$$absorption = \int_V \Sigma_a(\mathbf{r}) f(\mathbf{r},t)dV$$

Finally the leakage component can be derived by defining the *neutron current density vector **J**(**r**,t)* which measures the *net* flow of neutrons in any given direction.

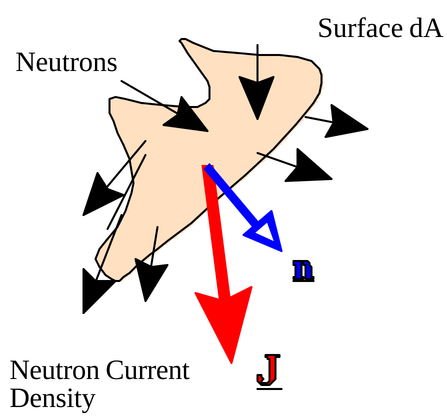

Figure 8-1 - Neutron Current Density

Let the vector ***n*** be a unit normal vector pointing outward from the surface *A* bounding *V*. The leakage rate from *V* is then:

$$leakage = \int_A \mathbf{J}(\mathbf{r},t) \bullet \mathbf{n}\,dA$$

Transforming this last equation from a surface to a volume integral, the continuity equation becomes:

$$\frac{d}{dt}\int_V n(\mathbf{r},t)dV = \int_V s(\mathbf{r},t)dV - \int_V \Sigma_a(\mathbf{r})\phi(\mathbf{r},t)dV - \int_V \nabla \bullet \mathbf{J}(\mathbf{r},t)dV$$

Since these are all over the same volume, we can remove the integral to get a point form of the *equation of continuity*:

$$\frac{\partial n(\mathbf{r},t)}{\partial t} = s(\mathbf{r},t) - \Sigma_a(\mathbf{r})\phi(\mathbf{r},t) - \nabla \bullet \mathbf{J}(\mathbf{r},t)$$

Fick's law states that the *current density vector is proportional to the negative gradient of the flux*. The proportionality constant is called the *diffusion coefficient*, *D.* Thus

$$\mathbf{J} = -D\vec{\nabla}\phi$$

The continuity equation, for uniform systems with a single neutron velocity *v* (so that $\phi = nv$), becomes the *neutron diffusion equation*:

$$D\nabla^2\phi - \Sigma_a\phi + s = \frac{1}{v}\frac{\partial \phi}{\partial t}$$

Transient neutron diffusion, plus kinetics, is the basis of many of the physics codes used in accident analysis. These equations are solved with spatial finite differences

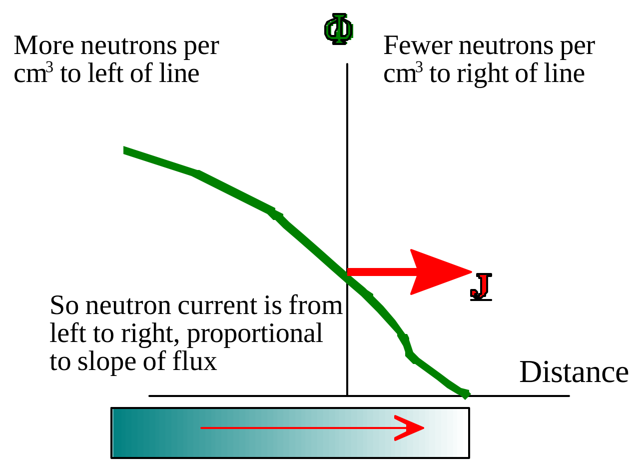

Figure 8-2 - Illustration of Fick's Law in 1D methods, with the reactor core broken up into many nodes, in each of which the diffusion equation is applied at each time step.

For a LOCA, for example, time-dependent cross sections representing the coolant voiding transient, fuel temperature transient, reactor control system action, and shutoff rod movement are the driving functions for the transient in the flux. The average power transient for the reactor is extracted from the calculation, along with peaking factors for the hot channel, hot bundle and the hot element in the loop being analyzed. The system reactivity as a function of importance-weighted[a] void fraction is also calculated. These data are used as input to a system thermohydraulics code. This code calculates the distribution of coolant void as a function of time from the pipe break, for each pass of the coolant loop. The importance-weighted average void fraction calculated by the thermohydraulics code is combined with the pre-calculated reactivity function, and the cycle is iterated as necessary. Nowadays the thermohydraulics code and the physics code can be combined into one calculation so that manual iteration is not necessary.

Our model is still missing some information. We indicated in Chapter 5 that shutting down a reactor was not sufficient to remove all safety concerns: the *decay heat* must be removed. This heat comes from the radioactive decay of fission fragments, and obviously cannot be controlled. In principle it can be calculated from the power history: the composition of fission products can be predicted at any time, their half-lives and decay chains are known, so that:

$$P_d(t) = \sum_i n_i(t) E_i$$

where:

$P_d(t)$ is the power produced by all decaying fission products at time t
$n_i(t)$ is the number of atoms decaying per unit time of fission product i at time t
E_i is the average energy produced by the decay of each atom of fission product i.

This is more complex than it seems, because $n_i(t)$ will depend on the irradiation history, each fission product may have more than one decay chain (with different energies), and there are many fission products. In practice such a fundamental calculation is done as a reference assuming a rapid shutdown after equilibrium operation. In most cases, the evolution of the accident (since it is short) does not materially change the decay power, so that the fundamental calculation is fitted with a series of

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[a] Voiding in a high-flux region has more effect on neutron kinetics than voiding in a low-flux region, since the former case changes the speed and absorption of more neutrons. Hence local void is weighted by the local flux in order to get the core-wide effect..

exponentials; and the fit is added to the fission power predicted by the physics codes. In exceptional cases, such as an accident occurring during power manoeuvring, this will not be very accurate - but as with any analysis, an upper bound can be assumed (e.g., assuming the decay power appropriate to prolonged steady-state operation at the maximum operating power level prior to the accident). Such a tradeoff between simplified assumptions which give a conservative bound to an answer, and more realistic assumptions which require more sophisticated analysis tools, is very common in safety analysis. Since safety analysis resources, like all other resources, are finite, part of the art of safety analysis is in judging when to use bounding assumptions, and when to use realistic complex models. The difficulty is, of course, that bounding models may lead to unnecessary restrictions on operation.

Fuel

Reactor fuel varies widely among different reactor types - for example many research reactors still use uranium metal fuel plates. Most water-cooled power reactors have solid UO_2 fuel pins (UO_2 is chosen because of its corrosion resistance at high temperature in water) surrounded by metal sheaths (clad) which contain any gaseous fission products released from the UO_2. We shall thus restrict the discussion to uranium oxide fuel.

The key safety parameters related to fuel are:

- fuel sheath integrity
- fission product inventory in (and release from) the fuel, and
- fuel temperature

Prediction of fuel temperature in CANDU is important because it drives sheath temperature, and hence sheath integrity; because limited fuel melting can lead directly to fuel sheath failure; and extensive melting can lead to pressure-tube failure. Also release of fission products from the fuel increases with fuel temperature. Finally there is a reactivity feedback from fuel temperature, which is not very large nor important in CANDU (but much more important (and much larger) in LWRs).

During normal operating conditions, all fission products are formed within the fuel grains; they are trapped there (with the exception of a few which recoil directly into inter-grain and gas gaps) until they are released from the grains by diffusion. The volatile fission products which are released form a gas mixture inside the fuel sheath. It is useful to categorize fission products into three groups: (a) bound inventory, (b) grain boundary inventory, and (c) gap inventory (recall Chapter 1).

The gap inventory includes the fission product gases in the pellet dishes, in the pellet/clad gap and in the sheath end cap. If the fuel sheath fails, the gap inventory escapes quickly, the grain boundary inventory much more slowly, and the bound inventory even more slowly. At relatively low fuel temperatures the diffusion processes are very slow, so that almost all isotopes remain in the grains. (An exception to this occurs when uranium dioxide is exposed to air at moderate temperatures; in this case oxidation to higher states takes place and the grain structure is destroyed.. Much of the fission products are then released. Such a circumstance could occur after failure of an end-fitting and ejection of the channel contents into the reactor vault). As temperature and fuel burnup increase the amount of fission gas in the gap increases, to a maximum of about 10% for typical CANDU operating conditions.

At any given burnup, a larger fraction of the fission product gases is released near the center of the pellet, where the temperature is highest. All volatile fission products tend to migrate down the temperature gradient toward the outside of the pellet. Their diffusion is assisted by the fact that the pellet cracks under the influence of temperature gradient; this cracking increases with fuel burnup and center temperature. At high burnup (and relatively low initial sintered fuel density) a hole develops at the center of the fuel pellet.

In summary:
(a) at low burnup or temperature, nearly all fission products are trapped in fuel grains,
(b) fission products trapped at grain boundaries increases with temperature and burnup,
(c) the gas gap inventory increases steadily with fuel temperature and burn-up.

Fuel Element Temperatures

Heat conduction in one dimension is given by the equation[2]

$$Q = -kA\frac{dT}{dx}$$

where Q is the rate of heat transfer; A is the area through which heat is transferred; dT/dx is the temperature gradient; k is the thermal conductivity. In terms of heat flux, $q=Q/A$,

$$q = -k\frac{dT}{dx}$$

Generalizing to three dimensions, and assuming energy is being produced in the medium at a volumetric rate H,

(Rate of change of internal energy) = (rate of energy release into medium) - (rate of energy loss from conduction)

or

$$r\,c\frac{\P T}{\P t} = H + k\nabla^{2}T$$

where ñ is the density and c is the specific heat.

Consider one-dimensional steady-state heat conduction in a cylindrical fuel pin (Figure 8-3). In cylindrical co-ordinates,

$$\frac{d^2T}{dr^2} + \frac{1}{r}\frac{dT}{dr} = -\frac{H}{k_F}$$

where k_F is the fuel thermal conductivity. Integrating,

$$T(r) = T(0) - \frac{Hr^2}{4k_F}$$

giving the typical parabolic radial distribution of temperatures within an oxide fuel element as shown in Figure 8-3. We can apply the same method to the temperature drop $ÄT_S$ across the sheath (for which the internally generated heat H_s=0):

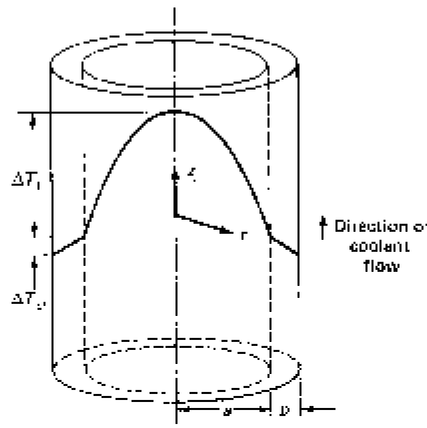


Figure 8-3 Fuel Temperature Distribution

$$\Delta T_S = T_{Si} - T_{So} = \frac{Ha^2 \log[(a+b)/a]}{2k_S}$$

where the indices *i* and *o* refer to the inner and outer surfaces of the sheath respectively. It would be tempting to conclude that the temperature drop from fuel centreline to the outer part of the sheath is just $ÄT_F$ +$ÄT_S$. Not so - the gap between fuel and sheath (not shown in Figure 8-3) provides a further thermal resistance, so we can write:

$$q = h_g\,(T_F - T_{Si})$$

where h_g is the gap heat transfer coefficient, determined from experiment.

The relationship between sheath and coolant temperature can be again derived from:

$$q = h(T_{So} - T_C)$$

where q is the heat flux per unit area to the coolant; T_C is the coolant temperature; h is the convective heat transfer coefficient. At steady state, all the heat produced in the fuel is transferred to the coolant, so that for a length of element *R*,

$$q = \frac{Hp\,a^2\ell}{2p\,(a+b)\ell}$$

so that

$$T_C - T_{So} = \frac{Ha^2}{2h(a+b)}$$

Typical values in CANDU fuel are:

k_F = 0.004 kW/m.°C
k_S = 0.017 kW/m.°C
h_g = 7 - 60 kW/m^2.°C
a = 6.07 mm
b = 0.42 mm.

Heat capacity does not enter the steady-state equations, but is important in transients. The values for uranium dioxide and Zircaloy-4 are, respectively, 0.5 and 0.4 J/g-°C. The corresponding heats of fusion are 27 and 42 J/g. The relatively large value of c and the high melting point (2840C) for UO_2 represent important safety characteristics: typically one can almost double the stored energy, relative to the normal operating point, inside UO_2 before it melts. Metal fuel, on the other hand, has little heat capacity and melts at a lower temperature; but has much higher thermal conductivity, typically ten times larger than UO_2.

Gas Pressure Inside Sheath

CANDU fuel has a "collapsible" fuel sheath, which creeps down plastically onto the pellet during irradiation due to the excess external coolant pressure. The small enclosed gas space in the element results in a high sensitivity of gas pressure to fuel sheath geometry. A small amount of fill gas is added to this space on assembly, so as to achieve the proper sheath stress distribution during operation. As burnup increases, the gas pressure causes the sheath once again to lift off the fuel; the gap heat transfer coefficient decreases because the sheath creeps away from the fuel pellet. This decrease leads to higher peak fuel temperature, greater fission gas release from the fuel, and finally higher gas pressure. A new equilibrium point is reached.

In accident analysis, fuel codes must have good models of the transient behaviour of the gas gap, since it is the driving force for sheath strain.

Fuel Behaviour in Accidents

During normal operation a CANDU 6 core contains 4560 fuel bundles, each with its unique conditions of location, burnup, and power level. On initiation of accident conditions each will behave differently depending on these parameters and the specific circumstances of the accident sequence. The end objective of in-core accident analysis is to estimate the quantity, characteristics, and timing of fission products released to the containment space. Obviously, a number of approximations will be required to obtain an estimate of this release. To introduce this topic, consider the effects on fuel of three abnormal conditions which might be encountered during an accident; (a) overpower, (b) low coolant flow, and (c) loss of coolant.

Overpower

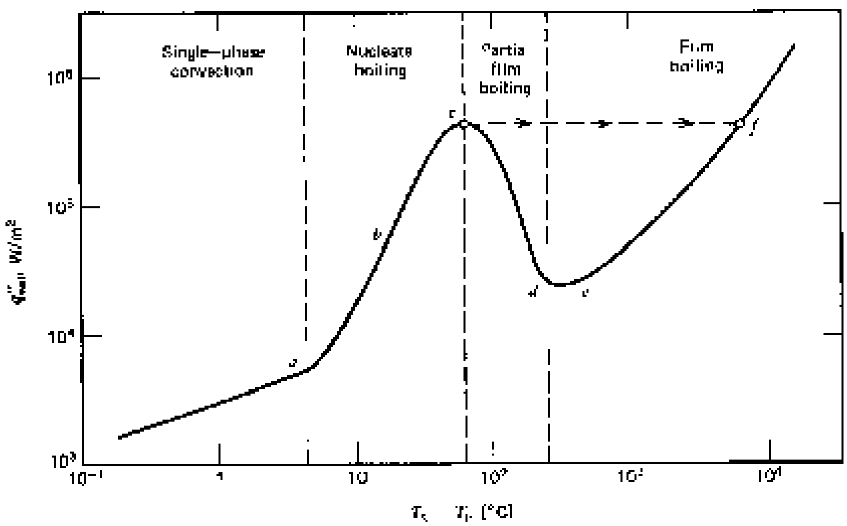
Sheaths might fail due to internal gas pressure or impingement of molten fuel, if the overpower is severe. The equation for the steady-state power level at which centerline melting begins can be derived from the radial heat conduction equation above, setting

$$T(0)=T_{melt}=2840\text{C}.$$

If a sudden power increase is imposed, so that there is no time for additional heat removal, the melting point is reached when an amount of energy is added given by $C_F(T_{melt}-T)$ for a local fuel volume, where C_F is the heat capacity.

Experiments in pulsed test reactors have been conducted to determine the fuel stored energy levels (when suddenly inserted) which lead to element rupture; in general, these are somewhat lower than those required to produce gross melting, especially for highly irradiated fuel.

In severe overpower transients, the fuel rod can be destroyed due to the formation of UO_2 *vapour* in the centre of the fuel; the vapour pressure blows the element apart. This was originally a concern for control rod ejection accidents in light-water reactors; the threshold for such breakup was established by the power burst tests mentioned above. It is likely that in Chernobyl the power pulse was sufficient to vaporize part of the fuel. It is not relevant for design basis accidents in CANDU.



Heat flux versus temperature difference for pool-boiling heat transfer.

Figure 8-4 - Boiling Curve

Dryout

This term is used loosely to identify a sudden drop in sheath to coolant heat transfer coefficient which occurs when a “critical heat flux” is exceeded. Figure 8-4 shows[3] the characteristic shape of the convective heat transfer curve for water as a function of surface heat flux; this curve is drawn for saturated liquid conditions in the fluid. On dryout, the sheath surface temperature jumps suddenly to the value at which the temperature change from sheath to coolant is sufficient to transfer the heat under the new film boiling flow regime. In water under the conditions of pressure, enthalpy, and flow typical of a modern PWR, this temperature change can be very large - dryout is roughly equivalent, under these conditions, to “shutting off” the heat transfer from fuel to coolant, and is often called “burnout”. Recalling Figure 8-3, with zero heat transfer the temperature distribution adjusts rapidly to a constant value approximately equal to the average fuel temperature before dryout. This average is about 1000C.

The effect of dryout is strongly dependent on the heat transfer regime of the coolant. Figure 8-5 shows the various regimes as functions of surface heat flux and thermodynamic quality. This Figure represents a tube heated from the outside with flow on the inside. Occurrence of the Film Boiling regime indicates a dry sheath (wall) surface. The heat flux is assumed constant along the tube.

Vigorous saturated nucleate boiling occurs as the average quality increases, thereby producing high turbulence. As a result the flow regime switches to annular, with a liquid film on the surface from which evaporation takes place to the vapour core. On transition to film boiling the liquid is driven off the surface, leaving a layer of vapour. The liquid droplets then travel in the vapour flow until they eventually evaporate due to heat transfer directly from the vapour. When the quality reaches unity, heat transfer continues to superheated vapour in single-phase flow. From our point of view, the most interesting

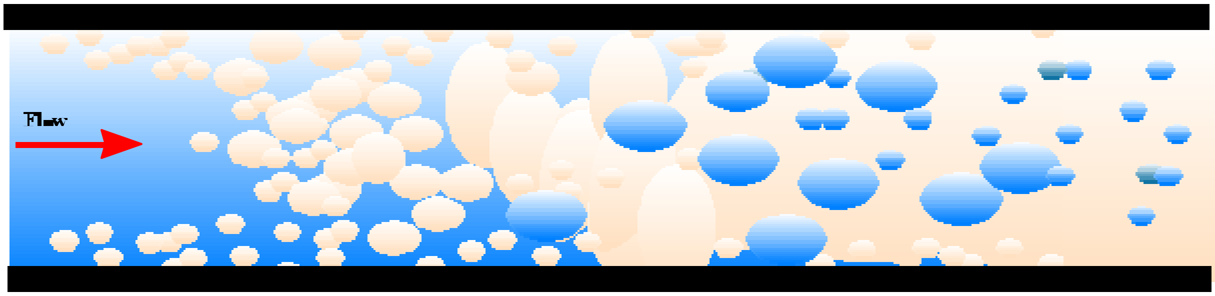


Figure 8-5 - Flow Patterns in a Heated Channel

transition is the one to film boiling, because it is here that the fuel sheath temperature may increase abruptly.

Dryout in a CANDU channel is not the same as in a PWR. PWRs run highly subcooled, so that dryout[b] occurs at low quality (mass fraction of steam) and at low steam velocities - thus the clad temperature rises rapidly. Most CANDUs, however, are designed so that in normal operation there is a small amount of boiling (typically <4% quality - note that the void fraction, obviously, is higher than the mass fraction). Dryout in a CANDU channel therefore tends to occur when the void fraction is high, so that there is a high steam flow-rate which provides reasonable post-dryout heat transfer. This fact is very important to the setting of safety system trip margins - it means that it is relatively *unimportant* if limited dryout occurs somewhere in the core. Trip setpoints therefore can be set somewhat higher.

The progressive effects of sheath dryout via overpower are listed below: the timing, endpoint, and eventual consequences of this sequence are strongly dependent on the details of the accident sequence being analyzed.

Overpower:
- Dryout
- Sheath temperature rise
- Zircaloy annealing

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[b]One can distinguish Critical Heat Flux (CHF), which is the onset of a dry spot on the sheath, from classical dryout, where the temperature takes a sharp jump

- Oxidation embrittlement of sheath
- Beryllium braze melting and attack on Zircaloy
- Zirconium-water reaction (exothermic)
- Bundle collapse
- Sheath melting
- Fuel melting (extremely unlikely)
- Pressure tube balloon or burst
- Heat transfer to moderator

Low Coolant Flow

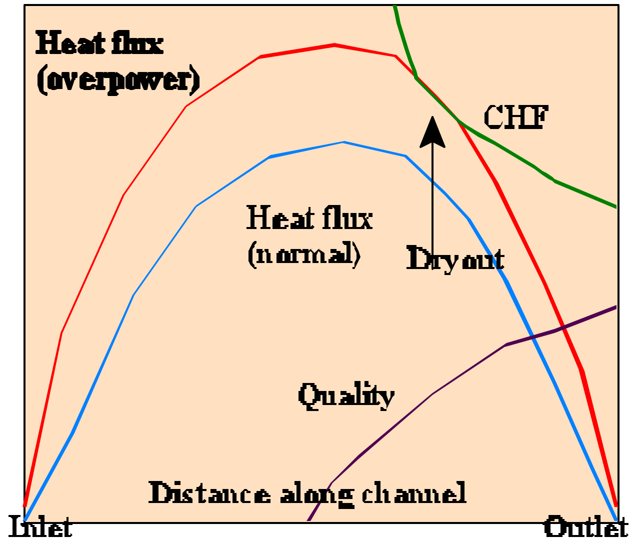

Figure 8-6 - CHF in CANDU Channel

This type of accident is expected to occur once or more in the plant lifetime. The most common cause is a loss of forced circulation, either due to a loss of Class IV electrical power or due to a single pump trip or seizure. In a single channel, flow reduction could be due to debris in the channel, or to a break in the inlet feeder. As in the overpower case, there is a flow/power mismatch; that is, more power is being produced in the fuel than can be removed by the coolant. The physical phenomena in the two cases are quite similar. Progressive effects of loss of flow are listed below.

Low Coolant Flow:
- Large increase in exit quality
- Heat Transport System overpressure (if the loss of flow is system-wide)
- Dryout
- Similar remaining sequence as for overpower

Loss of Coolant

This case has characteristics similar to both overpower and low coolant flow. Depending on the location and size of the pipe break, low flow occurs in some subset of the coolant channels in the core. Loss of coolant results in a system low pressure, with resultant flashing of water in the channels. The increase in quality leads to dryout and fuel overheating. The reactor power also rises initially due to the positive coolant void reactivity.

Large Loss of Coolant:

- Rapid decrease in local saturation temperature
- Flashing (rapid boiling) proceeds upstream from channel exit
- Neutron overpower due to coolant voiding (terminated by shutdown)
- Same fuel sequence as for overpower plus effect of sheath strain
- Heat Transport ystem pumps avitate when ressure is about qual to saturation ressure at the pump let - flow drops apidly

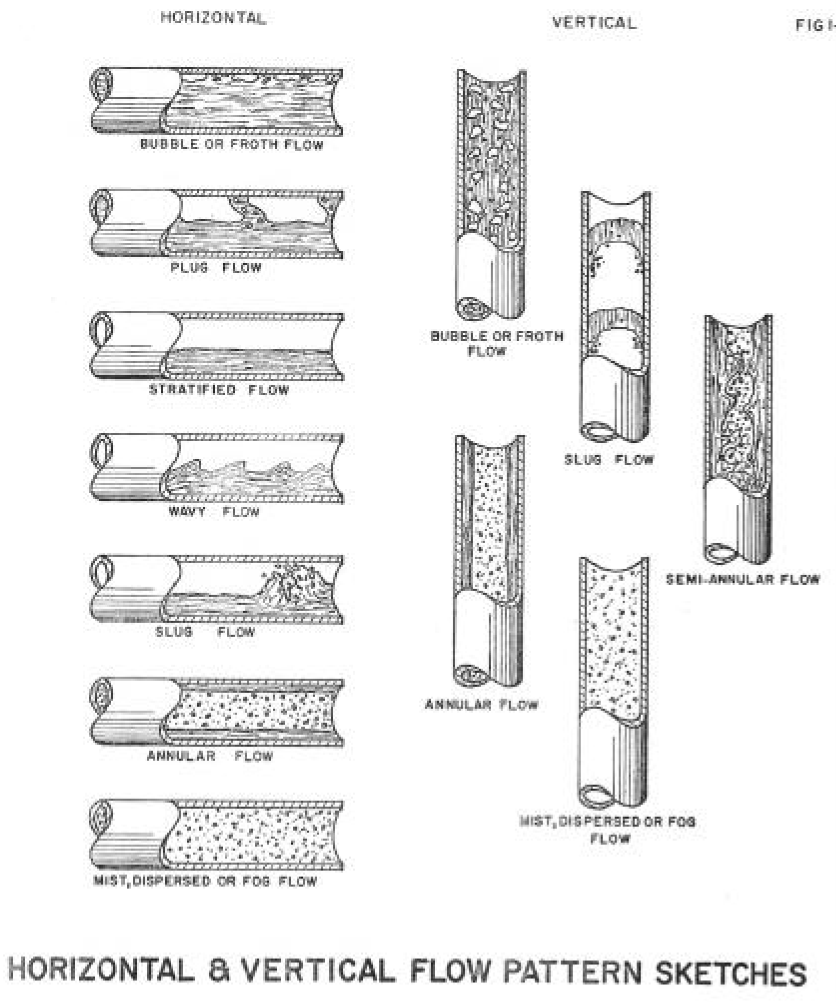

Figure 8-7 - Flow Regimes - from J.T. Rogers

S c p e p in r

b c i L L c in lo m B a fl in p s w g al a

In some accidents channel ehaviour under low flow onditions becomes mportant - e.g. small OCA just prior to trip; all OCAs under low flow onditions once ECC has itiated; and the intact HTS op post-LOCA, after the ain HTS pumps are tripped. ecause CANDU channels re horizontal, under low ow conditions, particularly two-phase flow, it is ossible for the flow to eparate into steam and ater under the influence of ravity, so that steam flows ong the top of the channel nd water along the bottom. This obviously affects cooling of the upper pins in the fuel bundle. The onset of such *flow stratification* is determined either from the fundamental two-fluid codes or more usually using empirical correlations. Figure 8-7 (from J.T. Rogers) shows examples of stratification along with more complex flow regimes in horizontal and vertical pipes. A similar situation obtains in the horizontal headers, although the flow regime is much more complex.

Fuel behaviour is more complex for a LOCA since the coolant pressure is decreasing. Since the fuel is generally heating up, this increases the gas pressure inside the sheath relative to the coolant pressure, and can force the sheath to strain. A uniform strain of at least 5% will not lead to sheath failure; however greater strains can lead to local instability, ballooning, and failure (these phenomena are less likely in CANDU because it takes very little sheath strain to relieve the gas pressure). The strain-rate equations are complex functions of material composition, material state, temperature, irradiation, and transverse stress, and are determined from experiments. Typically their form is as follows:

Define the *transverse stress* across the sheath as:

$$s = \frac{\mathrm{Pr}}{w}$$

where: P is the pressure differential across the tube
r is the tube radius
w is the tube thickness

The strain rate is then expressed in terms similar to the following:

$$\dot{e} = \frac{de}{dt} = As^{n}e^{-k/T} + Bs^{m}e^{-\ell/T}$$

where A, B, k, l, m, n are determined from experiment; and T is temperature.

In all of these situations, the pressure tube can be overheated via conductive, convective, and radiative heat transfer from the hot fuel. If the channel pressure is high, the pressure tube might burst; in most cases it will either balloon or sag to contact the calandria tube and transfer heat to the moderator water. The equations for pressure-tube strain are, not surprisingly, similar to those for sheath strain.

Heat Transport System

In brief, the behaviour of the heat transport system is predicted by solving the equations of mass, energy and momentum conservation for non-equilibrium transient two-phase flow in a network in one-dimension. "Two-phase" means that we consider steam and water. "Non-equilibrium" means that the steam and water phases, even in the same location, can have different pressures, temperatures, and flowrates. “Transient” means obviously that we want the behaviour as a function of time. Current CANDU codes are one-dimensional, although sometimes phenomenological two- or three-dimensional models are used for components such as headers. This limitation to one dimension is less of a problem for CANDUs than it is for LWRs, with their large pressure vessel; thus 2D and 3D codes *have* been developed for LWRs. “Network” means we model parallel paths (e.g., fuel channels, ECC) and several components connected together at the same point (e.g., at the headers).

Much effort in developing codes to model the heat transport system lies in the following areas:
- equations of state for the various phases
- component models for steam generators, fuel channels, fuel, headers, secondary side, valves, pumps etc.
- correlations for pressure-drop, heat transfer (including CHF), flow regimes
- efficient numerical solution schemes
- plant controllers

Most thermohydraulic simulation codes for reactors break the circuit up into nodes containing mass and therefore energy, and links joining the nodes, characterized by flow, length, roughness, diameter etc. Mass and energy conservation equations are written for the nodes, and the momentum equation is

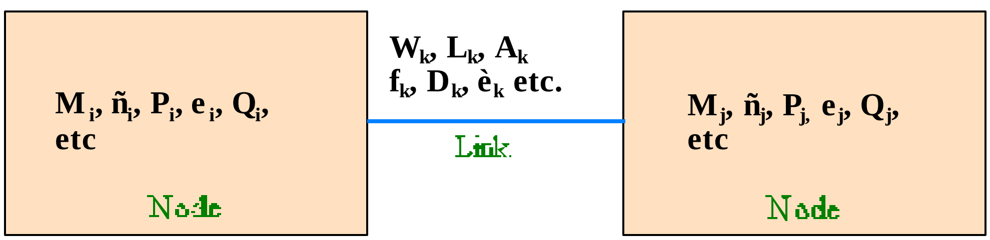

Figure 8-8 - Link/node structure of thermohydraulics codes

written for the links. We shall show simplified examples here (one dimensional flow in a level pipe).

Thus the mass conservation equation for node *i* is:

$$\frac{dM_i}{dt} = \sum_k W_k$$

where W_k are all the mass flows into and out of node i from links k.

The conservation of momentum equation is applied to link k and is (ignoring gravity):

$$\frac{dW_k}{dt} = \frac{A_k}{L_k}\left[(P_i - P_j) - \left(\frac{f_k L_k}{D_k} + k_k \right) \frac{W_k^{\,2}}{2 g_c r A_k^{\,2}} \right]$$

where for the link:

W is the mass flow in link k (in the picture, between nodes i and j)
A is the flow area
P is the pressure in the nodes connected to the link
L is the length
D is the hydraulic diameter
$(fL/D + k)$ is the friction factor

The first term is just Newton's law applied to a fluid to which a pressure difference is applied; the second term is the loss due to friction. Terms for pumps and gravity can be added.

The conservation of energy is applied to each node i as follows:

$$\frac{dU_i}{dt} = \sum W_{in} e_{in} - \sum W_{out} e_{out} + Q_i$$

where: U_i is the internal energy of node i
Q_i is the heat generated in node i

The summations are the rates of energies coming into and out of node i due to mass transfer.

These three equations are applied to each phase. There are four unknowns, e.g., mass, momentum, temperature and pressure. The fourth equation needed is the *equation of state* for each fluid, typically in the form of

$$r = f(P,T)$$

In safety analysis codes, the equation of state is used in the form of massive detailed tables of water and steam properties, or fitted by correlations.

Fuel Channels

When we look at behaviour of fuel channels in accidents, we emphasize three basic disciplines: heat transfer, stress-strain behaviour, and hydrogen chemistry.

Heat transfer

Heat can be transferred from the fluid to the pressure tube by conduction and convection; and from the fuel to the pressure tube by conduction (if it sags into contact with the pressure tube). At high temperatures, the fuel can transfer heat to the pressure tube by radiation, characterized by the Stefan-Boltzmann law,

$$E = es\left(T_f^4 - T_{PT}^4\right)$$

where g is the emissivity

T is temperature in degrees Kelvin

ó is the Stefan-Boltzman constant (1.36 $\times 10^{-4}$ kilo-calories per metre^2-second-K)^4

the subscript f refers to fuel and PT to pressure-tube

A similar equation would apply to radiation from the pressure-tube and from the steam itself, although these tend to be small.

In practice radiation becomes important at sheath temperatures around 800C or more and is about equal to the decay power in the fuel around 1200-1400C. Also in practice the hard part is working out the geometry: computer codes break the complex fuel bundle and pressure-tube into smaller pieces; calculate the “view factor” (how much of the pressure tube or neighbouring fuel element each piece can “see”) for each piece; and calculate the radiation heat transfer piece by piece.

Heat can also be transferred from the calandria tube to the moderator, which is significant after pressure-tube contact (see below). The heat transfer characteristics follow a pool boiling curve, similar in concept to Figure 8-4. Limited patches of film boiling can be tolerated for short periods after contact; lengthy or extensive dryout will lead to calandria tube failure.

Strain
If the pressure tube heats up in excess of 800C or so, it will start to plastically deform and/or sag until it either bursts or contacts the calandria tube. This has been discussed already. Generally at internal pressures less than about 6 MPa the pressure tube will strain uniformly to contact the calandria tube; at high pressures, it is more likely to rupture locally before contact.

Hydrogen
At high temperatures, Zircaloy oxidizes in steam to produce heat and hydrogen:

$$Zr + 2H_2O \Rightarrow \; ZrO_2 + 2H_2 + \; heat$$

This is a quadruple threat:

- the hydrogen collects in containment (significant amounts of hydrogen can only be produced by a LOCA with ECC failure[c]) and can, in the right circumstances, become flammable;
- the heat generated by the chemical reaction increases fuel and pressure tube temperatures;
- the presence of a non-condensible gas in large quantities can impede ECC water, if the operator tries to recover from an impairment of ECC by injecting water, late[d]; and
- the formation of oxide embrittles the sheaths and pressure tubes so that they may shatter if ECC is eventually restored.

Correlations of the reaction rate of steam and Zircaloy therefore form an essential part of fuel channel codes.

The reaction rate becomes autocatalytic around 1400-1500C - that is, the heat it generates keeps the chemical reaction going with no further heat input, much like a fire. In US reactors, this is a major concern: the fuel elements are close together, so there is no place for the heat to radiate to. Thus US regulatory practice sets a strict limit on sheath temperature in a design basis accident - namely 1200C - chosen so that there is little possibility of an autocatalytic reaction. In CANDU, the presence of the cold

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[c](Footnotes are for caveats): Hydrogen can also be produced slowly in the long term by radiolysis (radiolytic decomposition) of ECC water as it circulates through the core.

[d]This was the fear behind the ‘gas bubble’ *within* the reactor vessel during the Three Mile Island accident. The hydrogen which escaped to containment formed a flammable mixture of 9% hydrogen and did indeed burn without serious consequences.

pressure tube less than a few centimetres from each fuel element moderates the reaction; embrittlement is still a concern but the regulatory practice permits calculation of actual oxidation rates and thicknesses, rather than setting a criterion based on temperature alone.

Moderator

The safety issue with the moderator is to predict the transient local water temperature at each point. The objective is to show that the local moderator subcooling at any location where the pressure-tube contacts the calandria tube in an accident is sufficient to prevent prolonged film boiling on the outside of the calandria tube. The physical problem is therefore solution of three-dimensional fluid flow with heat addition in a porous medium - the medium is not continuous because of the presence of fuel channels, reactivity devices, etc. The mass, momentum and energy equations described above are therefore generalized to three dimensions. Experimental validation is of course a must, because of the complex geometry.

Moderator chemistry is another area of interest. In normal operation, the moderator contains dissolved deuterium gas and oxygen gas from the radiolysis of heavy water[e]. Gases which come out of solution are normally recombined in the gas steam taken from the cover gas space above the moderator level; however chemistry upsets can cause the gases to come out of solution quickly with the potential for burning or exploding (if there is an ignition source, which normally there is not). This is of particular interest when the cover gas is open for maintenance since then there can be ignition sources.

In addition the gadolinium nitrate used in Shutdown System #2 can precipitate if the chemistry becomes unfavourable.

Both such events have actually occurred, without any plant damage.

Containment

As far as fundamental equations are concerned, containment behaviour is governed by the same physics as the heat transport system, with a few complications:

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[e] $2D_2O + radiation \leftrightarrow 2D_2 + O_2$

1. the containment volume is usually compartmentalized and the flow within the larger compartments is three-dimensional;
2. there are a number of different fluids coexisting: air (normal contents of containment), steam and water from a pipe break, and hydrogen if the sheaths are heavily oxidized;
3. heat is added by the steam and hot water, and also by the radioactive decay of any fission products carried into the containment atmosphere by the discharging fluid; heat is removed by dousing (water sprays), condensation on containment and equipment surfaces, and by containment air coolers
4. the pressure can also be influenced by: use of the vacuum building (in multi-unit plants), leakage from containment through cracks, and by deliberate venting through filters.

Containment codes usually have sub-models for each of these phenomena.

Many containment codes also track the movement of fission products along with the other fluids. Fission products can exist as
1. noble gases, which interact very little with water or surfaces;
2. tritium oxide (specifically the mixed oxide DTO), from the coolant or moderator. Obviously tritium oxide behaves similarly to steam and/or water, from the break or leak. It will leak through cracks but is far more likely to remain in the building in pools or on wet surfaces;
3. iodine, caesium, strontium, etc. which interact strongly with water (dissolve) and tend to plate out on surfaces;
4. actinides such as plutonium. These are released from the fuel in quantity only if the core is massively destroyed.

Generally iodine-131 is the significant radioisotope of concern because of its short half-life (8.1 days), high-energy gamma emission, and ability to get into the food chain through the following route:

- released from containment
- deposits on grass
- eaten by cows
- excreted in milk
- drunk by people.

The external (direct) dose from atmospheric release of iodine-131 can also be significant.

Fortunately, as long as the pH of water inside containment is high, iodine will stay dissolved in it. This is easy to design for: for example on concept developed by AECL proposed that bags of tri-sodium-phosphate were to be stored in the reactor building basement; in an accident, they get flooded, the TSP dissolves, and keeps the pH high.

Figure 8-9 from D. Meneley summarizes this discussion..

FIGURE 1.1 – Fission Product Behaviour under Accident Conditions

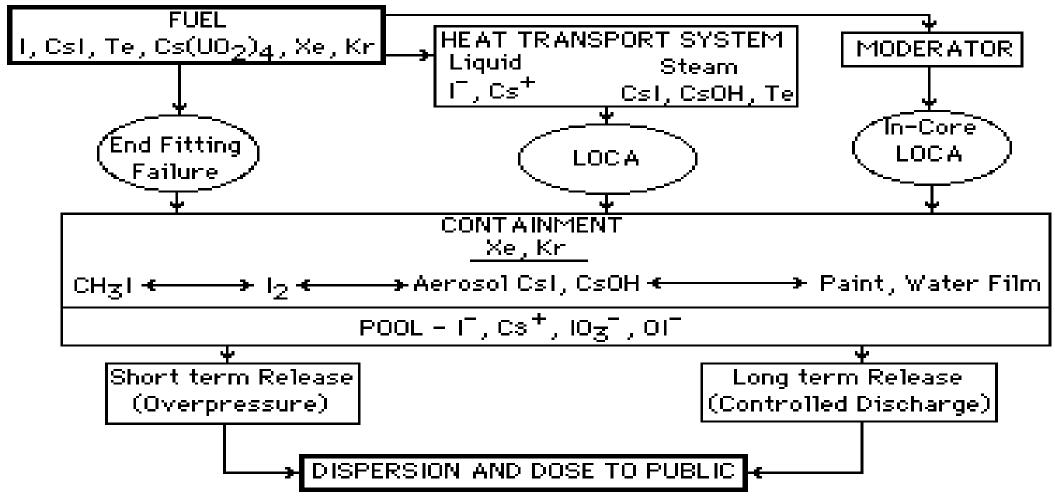

Figure 8-9

Fission Products, Atmospheric Dispersion and Dose

Fission Product Source Term

The fission product inventory in an operating reactor can be estimated as follows[4]. Suppose that the reactor has been operating at a power of *P* MW. If the recoverable energy per fission is taken to be 200 Mev, the total number of fissions occurring per second is

$$\begin{aligned}\text{Fission rate} &= P\ \text{MW} \times \frac{10^{6}\text{joule}}{\text{MW}-\text{sec}} \times \frac{\text{fissions}}{200\text{Mev}} \times \frac{\text{Mev}}{1.60\text{x}10^{-13}\text{joule}} \\ &= 3.13 \times 10^{16}\ P\ \text{fissions/sec.}\end{aligned} \tag{1}$$

If the cumulative yield of the ith fission product (the yield of the fission product itself plus the yields of all its short lived precursors) is γ_i atoms per fission, then the rate of production of this nuclide is

$$\text{rate of production} = 3.13\text{x}10^{16}\, P\, \gamma_i \ \text{atoms/sec.} \tag{2}$$

The activity at time *t* of that fission product while in the core of the reactor is

$$\alpha_i = 3.13\text{x}10^{16}\, P\, \gamma_i \left(1-e^{-\lambda_i t}\right) \text{disintegrations/sec.} \tag{3}$$

Expressed in Curies, this is

$$\alpha_i = 3.13\text{x}10^{16}\, P\, \gamma_i \left(1 - e^{-\lambda_i t}\right) \text{disintegrations/sec. x } \frac{1 \text{ Ci}}{3.7\text{x}10^{10} \text{dis./sec.}}$$
$$= 8.46 \text{ x } 10^5\, P\, \gamma_i \left(1 - e^{-\lambda_i t}\right) \text{ Ci} \quad (4)$$

(If you feel more at home in Becquerels, remember that 1 Bq = 2.7 x 10^{-11} Ci, and 1 TBq = 10^{12} Bq or 27 Ci. So to get this in TBq, divide by 27).

If the activity saturates in the time, t, that is, if $\lambda_i >> 1$, equation 5 reduces to

$$\alpha_i = 8.46 \text{ x } 10^5\, P\, \gamma_i \text{ Ci} \quad (5)$$

Figure 8-10 gives the inventories of the most important noble gases and iodine fission products computed for a typical 1000 MWe (PWR) plant at the end of a fuel cycle.

The amount of a fission product available for release to the atmosphere can be estimated by

$$C_0 = 8.46 \text{ x } 10^5\, F_p F_b P\, \gamma_i \left(1 - e^{-\lambda_i t}\right) \text{ Ci}, \quad (6)$$

where F_p is the fraction of the radio nuclide released from the fuel into the reactor containment and F_b is the fraction of this that remains airborne and capable of escaping from the building.

Typical core inventory of selected volatile fission products in a 1000 MWe PWR at the end of a fuel cycle

Nuclide*	Half-life†	Fission yield‡	Curies ($\times 10^{8}$)§
^{85m}Kr	4.4 h	0.0133	0.24
^{85}Kr	10.76 y	0.00285	0.0056
^{87}Kr	76 m	0.0237	0.47
^{88}Kr	2.79 h	0.0364	0.68
^{133}Xe	5.27 d	0.0677	1.7
^{135}Xe	9.2 h	0.0672	.34
^{131}I	8.04 d	0.0277	.85
^{132}I	2.28 h	0.0413	1.2
^{133}I	20.8 h	0.0676	1.7
^{134}I	52.3 m	0.0718	1.9
^{135}I	6.7 h	0.0639	1.5

*Superscript *m* refers to a nuclide in an isomeric state (see Section 2.8).
†m = minutes, h = hours, d = days, y = years.
‡Cumulative yields in atoms per fission; equal to yield of nuclide plus cumulative yield of precursor. From M. E. Meek and B. F. Rider, "Compilation of Fission Product Yields," General Electric Company report NEDO-12154, 1972.
§From "Reactor Safety Study" WASH 1400, 1975.

Figure 8-10

Atmospheric Dispersion

Consider a reactor containment after an accident, in which the concentration of a particular nuclide is C Bq/m^3. Assume a leak rate of V m^3/ s into the atmosphere at a height h metres as shown in Figure 8-11 . The release rate Q is given by:

$$Q = C\ (\mathrm{Bq/m^3})\ \mathrm{x}\ V\ (\mathrm{m^3/s}) = C\ V\ (\mathrm{Bq/s}) \tag{7}$$

This release is dispersed into the surrounding area via the release plume. For a given weather condition with wind velocity *u* and other data, a concentration of radioactivity at some distance and direction from the source can be calculated from:

$$\chi = \left(\frac{2}{\pi}\right)^{1/2} \frac{Q}{\sigma_z \bar{u}} \frac{f}{\theta x} e^{-h^2/2\sigma_z^2} \tag{8}$$

where:

÷ is the sector-averaged long-term concentration in Bq/m^3 a distance *x* metres from the source, and will be uniform through the sector

Q is the release rate in Bq/s from a source *h* metres in height

ó$_z$ is the vertical diffusion coefficient in metres

è is the angle subtended by the sector [radians]

f is the fraction of time the wind blows into the sector

$\overline{u}$ is the mean wind velocity in m/s.

This is the so-called *Gaussian* dispersion model.

Dose

The local radiation leads to an external dose (often called ‘cloud’ dose) due to the ambient radiation level and an internal dose due to inhaled species. By way of example, iodine production at McMaster for use in medical applications generates Ar^{41}, which is a source of external dose, and I^{125}, which is a source of internal dose. In contrast to I^{131}, the â-ray from I^{125} is too soft to be much of an external risk since clothing and the outer dead layer of skin provides shielding. Inhalation, however, leads to direct exposure to tissue. This is aggravated since iodine is readily absorbed by the body and concentrates in the thyroid gland. External dose, then, is a function of the time exposed to an ambient radiation level. Internal dose is a function of the radiation uptake and the residence time in the body.

For the external case using Ar^{41} as an example, 1 Bq/m^3 gives a dose of 2.3x10^{-10} Sv/hr. Thus:

$$\text{Dose}_{\text{external}}\ [\text{Sv/yr}] \ ' \left(Q\ \frac{\text{Bq}}{\text{s}}\right)\left(÷/Q\ \frac{\text{s}}{\text{m}^3}\right)\left(2.3\text{x}10^{\&10}\frac{\text{Sv/hr}}{\text{Bq/m}^3}\right)\left(24\text{x}365\ \frac{\text{hr}}{\text{year}}\right) \tag{9}$$

A typical dilution factor (÷/Q) is 4.5x10^{-6} s/m^3 at 200 metres from a release at a height of 20 metres, which gives a dose of 9.1x10^{-12} Q Sv/yr. A dose limit of, say, 5 mSv/yr gives a release limit of .005 / 9.1x10^{-12} = 5.5x10^8 Bq/s. Equation 8 can then be used to infer a limit on the permitted concentration in the building.

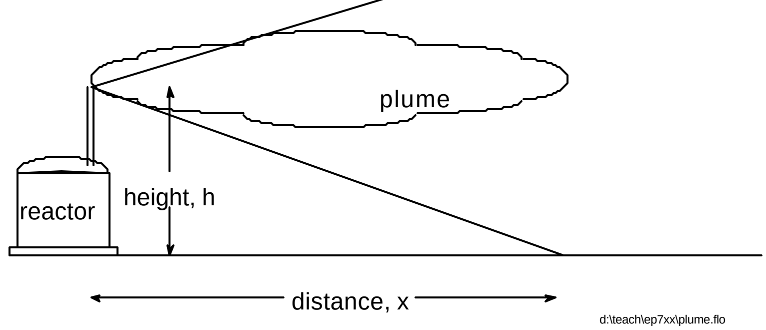

Figure 8-11 - Atmospheric Dispersion Parameters

For internal uptake of I^{125}, 1 Bq leads to $2\text{x}10^{-6}$ Sv. This is due to the integrated dose received, which is a function of the dose level (Bq/time) and the residence time. The uptake rate is just the inhalation (volume) rate which is roughly 3.8 m^3/day for an infant. The dose is thus:

$$\begin{aligned} \text{Dose}_{\text{internal}}\ [\text{Sv}] &= \left(Q\ \frac{\text{Bq}}{\text{s}}\right) \left(\div/Q\ \frac{\text{s}}{\text{m}^3}\right) \left(3.8\ \frac{\text{m}^3}{\text{day}} \text{ x } 365 \frac{\text{days}}{\text{year}}\right) \left(2\text{x}10^{-6}\ \frac{\text{Sv/yr}}{\text{Bq}}\right) \\ &= \text{release rate x dilution factor x volume rate x dose/uptake} \\ &= \text{local concentration x volume rate x dose/uptake} \\ &= \text{uptake x dose/uptake} \end{aligned} \tag{10}$$

Using the same dilution factor of $(\div/Q) = 4.5\text{x}10^{-6}\ \text{s/m}^3$, the internal dose is $1.248\text{x}10^{-8}$ Q Sv. Thus a dose limit of 10µSv is received for a release of

$$Q\ [\text{Bq/s}] = \frac{10\text{x}10^{-6}\text{Sv}}{1.248\text{x}10^{-8}\text{Sv/(Bq/s)}} = 801\ \text{Bq/s} \tag{11}$$

Details can be found in Canadian Standards Association Standard CSA-N288.1.

Acknowledgement

Much of the material in this chapter was based on lectures by D. Meneley. His permission to use them is gratefully acknowledged. I have also used some good diagrams from T. Rogers.

Exercises

1. Calculate the average volumetric heat generation of the fuel in a 600MW CANDU at 100% power. At what percentage power (assuming the same heat removal from the fuel as in normal operation) would the centre of the average pin melt?

2. Calculate the dose due to the release of 1000 Ci of Xenon-133 from a CANDU. Assume the release is at 20m.high, and the receptor is 1 km. distant. Consult CSA-N288.1 for any models you need; assume a 'reasonable' dispersion factor as above.

3. Calculate the dose due to the release of 1000 Ci of Iodine-131 from a CANDU. Assume the release is at 20m.high, and the receptor is 1 km. distant. Consult CSA-N288.1 for any models you need; assume a 'reasonable' dispersion factor as above.

4. How many grams does 1000 Ci of iodine-131 represent? (Hint: remember the half-life).

5. Calculate: (a) the amount of hydrogen produced by oxidation of 25% of the Zircaloy in the sheaths in a CANDU (this is not untypical of a severe accident such as a LOCA + LOECC); (b) the amount of energy released (you will need to look up the heat of reaction). (c)Assume this energy is released starting from 30 minutes after the accident and ending two hours afterwards. Compare the energy to the decay heat produced in the same time. (d) Now assume the hydrogen is transported into containment and burns. Calculate the energy produced by the burn. (e) Assuming the containment is a cylinder 40m. high and 40m. in diameter, and that at the time of the hydrogen burn it is filled with air and steam at a pressure of 15 psig and a temperature of 120C, calculate the increase in containment pressure (you will need to estimate the mass of air and water in containment). (This exercise would make a good project)

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