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Salination and Desalination of D<sub>2</sub>O in the SNO Detector

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## 1. Introduction

It is proposed to alternate the operation of the detector with and without NaCl in solution at the level of 0.25%, with a periodicity of some months. During the processes of salination and desalination, and more generally and importantly during any period of inhomogeneity of the D<sub>2</sub>O saline solution, it may be difficult to interpret the data recorded, and for this reason it is desirable to minimize the change-over times.

The main purpose of this note is to assemble the numerical values of the various parameters which enter the problem and the few formulae of fluid dynamics which can be applied. The numbers relate to H<sub>2</sub>O as it is difficult to find a complete set for D<sub>2</sub>O and unlikely that D<sub>2</sub>O will be very different, apart from the numerical value of the density. The formulae have been taken from Landau and Lifshitz, Fluid Mechanics, Pergamon 1959, Third Impression 1966, pp6 to 9 and 212 to 215, apart from a minor modification for an inhomogeneous body of fluid, and the ASC report 90 1022 1. Numerical values are given in Appendix I, the formulae in Appendix II and estimates for SNO in Appendix III.

## 2. Properties of Water

The Appendices reveal a number of simplifying characteristics:

- a) Heat transfer must involve convection, conduction is far too slow.
- b) Diffusion is negligible on the time scales of interest.
- c) The compressibility can be largely ignored.
- d) Any negative temperature gradient is expected to induce turbulent convection, and therefore mixing.
- e) Concentration gradients are likely to be as important as temperature gradients for driving convection.
- f) The acrylic vessel is better approximated as a thermal insulator on a time scale of a few days, a conductor on a time scale of months.
- g) The electrical conductivity of salt solution suggests itself as a basis for monitoring the concentration and uniformity.

## 3. Steady State Operation

The predicted heat input to the 7000 tons of H<sub>2</sub>O plus 1000 tons of D<sub>2</sub>O is 10KW from the rock walls and 2KW from the photomultiplier bases, which will be balanced by the heat removed by the separate cooling systems on the H<sub>2</sub>O and D<sub>2</sub>O recirculation systems, respectively 150 and 100 l per minute. If the recirculation flows were to enter the vessel at 1°C below the equilibrium temperature then the H<sub>2</sub>O cooler would remove 10KW and the D<sub>2</sub>O cooler 7KW. The heat transfer within the bulk of the water is expected to be turbulent convective. In these circumstances most of the temperature drop between the heat sources and sinks can be expected to occur in the boundary layers with only a small, (but  $> 10^{-4}$ °C/m from the local stability conditions) temperature gradient within the main body of water. This gradient is most unlikely to be less than 10 °C per m in the pure H<sub>2</sub>O, the minimum necessary to satisfy the local condition

for convection (Appendix II), and  $10^{-4}^{\circ}\text{C}$  per m should be more than adequate to drive turbulent convection in the  $\text{D}_2\text{O}$ .

#### 4. Salination of $\text{D}_2\text{O}$

It is assumed that the NaCl will be stored as  $50 \text{ m}^3$  of 5% brine and can be introduced at the flow rate of the recirculation system, 100 l per minute, in about 8 hours. If the brine, at higher density and lower temperature than the  $\text{D}_2\text{O}$  in the acrylic vessel, enters the top of the vessel then turbulent convective mixing can be expected.

It is argued in Appendix III that the fluid dynamics within the  $\text{D}_2\text{O}$  will be effectively isolated by the acrylic vessel from the fluid dynamics of the  $\text{H}_2\text{O}$ . The convective time scale for a  $\Delta T = 1^{\circ}\text{C}$  is estimated (see ASC report) as some minutes, but as the time varies only as  $1/\sqrt{\Delta T}$  the actual value of  $\Delta T$  is uncritical.

It appears that the  $\text{D}_2\text{O}$  can be brought up from zero to 0.25% NaCl concentration by introducing  $50 \text{ m}^3$  of 5% NaCl concentration at  $-1^{\circ}\text{C}$  over 8 hours, and extracting  $50 \text{ m}^3$  with a mean concentration of 0.125%. Throughout the 8 hours the content of the acrylic vessel is expected to have a uniform concentration varying linearly with time.

#### 5. Desalination of $\text{D}_2\text{O}$

It is proposed to remove the 0.25% salt in the  $\text{D}_2\text{O}$  by reverse osmosis, ideally rejecting  $50 \text{ m}^3$  of the total of  $1000 \text{ m}^3$  as a 5% concentration of salt. Seven days at 100 l/min are required to process  $1000 \text{ m}^3$  and if no mixing occurs between the residue of the 0.25% residue in the acrylic vessel and the purified  $\text{D}_2\text{O}$  returned to the vessel then desalination will take just 7 days. If mixing does occur with a time constant  $\ll 7$  days then desalination will be exponential with a 7 day time constant.

The most favourable circumstance for mechanical stability, i.e. no mixing, is a positive temperature gradient and a negative concentration gradient, which could be achieved by pumping out the salt solution from the bottom of the acrylic vessel and returning the purified  $\text{D}_2\text{O}$  to the top of the vessel at a temperature a little higher, say  $+1^{\circ}\text{C}$ , than the temperature of the contents of the acrylic vessel. This is equivalent to a power input of 7KW for a flow of 100 l/min.

The estimates of Appendix III are very encouraging in the sense that it is most unlikely that convection (and therefore temperature gradient) and a negative concentration gradient are established, independent of the (small) temperature gradients which will occur in the  $\text{H}_2\text{O}$  and are insulated from the  $\text{D}_2\text{O}$  by the acrylic vessel.

#### 6. Conclusions

Recirculation of the  $\text{D}_2\text{O}$ , saline or pure, for steady state operation might best be carried out by alternating the temperature of the return flow to the top of the acrylic vessel between  $\pm$  a few tenths of a  $^{\circ}\text{C}$  relative to the content of the vessel with a periodicity of the odd day to ensure convective mixing (time constant of minutes) and therefore homogeneity, while maintaining a steady mean temperature (time constant of 7 days). Prior to the change, saline to or from pure, it would be appropriate to set up the required temperature gradient by returning the  $\text{D}_2\text{O}$  at  $\pm 1^{\circ}\text{C}$  for some days.

The salination can be expected to take  $\sim 8$  hours with the content of the acrylic vessel remaining homogeneous throughout, the return being maintained at  $-1^{\circ}\text{C}$  for the 8 hours.

Desalination will require 7 days with the return at  $+1^{\circ}\text{C}$ , plus a further 7 days at  $-1^{\circ}\text{C}$  to return the temperature to the desired value and ensure homogeneity through convective mixing. During the first 7 days the salt concentration of salt will be spatially inhomogeneous but possibly well defined. Presumably homogeneity will be fully restored in a fraction of a day by the  $1^{\circ}\text{C}$  return.

A caveat must be entered with respect to turbulent convective mixing given the cautious approach of the ASC report despite the huge magnitude of the Grashof number. Landau and Lifshitz are less cautious, but doubt remains. If the heat transfer is indeed via laminar convection it is likely that a flow pattern of hexagonal cells will be formed, flow up the centre and down the sides of each hexagon. The time constant for mixing may then be determined by diffusion over a length with the magnitude of the dimension of a hexagon, which according to Landau and Lifshitz is a difficult theoretical problem. The mixing time constant could be long as the scale magnitude for diffusion of NaCl is an inch in a week, the distance varying as the square root of the time.

It will be necessary to monitor the concentration and homogeneity of the salt at least to the extent of sensors in the input and output pipework. Electrical conductivity looks the obvious technique and is simple enough that a sensing head might be mounted with a calibration source.

One final reservation should be mentioned concerning the local stability condition set up in Appendix II for inhomogeneous brine. The thermodynamics is incomplete to the extent that the chemical potential was ignored, but it is thought unlikely that this will change the qualitative features.

## Appendix I

## Numerical Values of Parameters

The numbers below all refer to H<sub>2</sub>O, not D<sub>2</sub>O, as it is difficult to find a complete set for the latter and it is unlikely that there could be an important difference between the fluid dynamics of H<sub>2</sub>O and D<sub>2</sub>O.

1. **Density** of NaCl solution is linear in % concentration  $c$  (g of NaCl per 100g of H<sub>2</sub>O).  $\frac{1}{\rho} \frac{d\rho}{dc} = 7.16 \times 10^{-3}$  per % at 20°C.
2. **Diffusion** of NaCl in H<sub>2</sub>O.  $D = 1.0 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$  at 10°C and 0.05 g mole per litre and is insensitive to concentration.  $\frac{1}{D} \frac{dD}{dT} = 0.025 \text{ K}^{-1}$ . Characteristic time for a distance of 6m is 10 years. Characteristic length for a time of 1 week is 24mm.
3. **Volume thermal expansion**.  $\beta = 210 \times 10^{-6} \text{ K}^{-1}$  at 10°C.
4. **Thermal conductivity** of H<sub>2</sub>O,  $K = 0.561 \text{ W m}^{-1} \text{ K}^{-1}$ . A power transfer of 10KW distributed over a circular area of 22m diameter (26.3W per m<sup>2</sup>) requires a gradient of 46.0 K per m.
5. **Electrical conductivity**  $\sigma$  of NaCl solution of concentration  $c$  % (see 1.) is nearly linear in  $c$  at low  $c$ ,  $\frac{d\sigma}{dc} = 1.14 \text{ ohm}^{-1} \text{ m}^{-1}$  per %. Temperature dependence  $\frac{1}{\sigma} \frac{d\sigma}{dT} = 0.025 \text{ K}^{-1}$  at  $c = 2\%$ .
6. **Viscosity**  $\eta = 1.307 \text{ mPa.s}$  at 10°C.  $\frac{1}{\eta} \frac{d\eta}{dT} = -0.029 \text{ K}^{-1}$  at 10°C.
7. **Compressibility**. Bulk modulus  $K = 2.05 \text{ GPa}$ . For a pressure increase of  $1.2 \times 10^6 \text{ Pa}$  the fractional increase in density is  $0.585 \times 10^{-4}$ , an increase which would also be achieved by a temperature reduction of 0.28K or a NaCl concentration of 0.008%.
8. **Specific heat**.  $C_p = 4.18 \text{ J/g/K}$   
Water recirculated at 100 l/min and cooled 1°C below the reservoir temperature corresponds to a power transfer of 6.7KW. The power associated with the kinetic energy of this water discharged through a pipe of 0.01m<sup>2</sup> cross-sectional area is  $2.3 \times 10^{-2} \text{ W}$ . If the recirculation cooler extracts 6.7KW, i.e. reduces the temperature 1°C, it will take a week to cool 1000 tons by 1°C, assuming the acrylic vessel is thermally isolated.
9. **Thermal Conductivity of Acrylic**  $K = 0.17$  to  $0.25 \text{ W m}^{-1} \text{ K}^{-1}$ .  
The acrylic vessel with a thickness of 5cm and surface area of 452m<sup>2</sup> will transfer  $4 \text{ W m}^{-2}$  and a total of 1.8KW for a 1°C temperature difference. The time constant for reducing the temperature difference by acrylic conduction is therefore 4 weeks.

## Appendix II

## Convection

Landau and Lifshitz give a number of relations concerning the mechanical stability of a fluid under gravity and the onset of laminar and turbulent convection. In particular they point out that if the temperature distribution is a function of the coordinates other than the vertical coordinate then mechanical equilibrium in the fluid is not possible, i.e. the fluid will exhibit macroscopic motion. (pp8 and 213).

For a fluid of uniform composition convection will occur for a temperature gradient,

$$\frac{dT}{dz} < -gT\beta/C_p = -1.4 \times 10^{-4} \text{ Km}^{-1} \text{ for water}$$

where  $g$  is the acceleration of gravity. In the case of a concentration  $c$  (of salt) which varies with  $Z$  it is necessary to modify the equations of Landau and Lifshitz (Section 4, pp 8,9). A fluid element of specific volume  $V(p,s,c)$  at height  $Z$  displaced (without mixing or heat conduction) to a height  $Z + dz$ , where the pressure is  $p'$ , entropy  $S'$ , and concentration  $C'$ , will have a specific volume  $V(p',s',c)$ , neglecting the small influence of  $p'-p$  on  $c$ , and displace an element of fluid of specific volume  $V(p',s',c')$ . The condition for convection is

$$V(p',s',c') - V(p',s,c) < 0$$

i.e.  $\frac{dV}{dZ} = \frac{\alpha V}{\alpha s} \frac{ds}{dZ} + \frac{\delta V}{\delta c} \frac{dc}{dZ} < 0$  which gives, ignoring any influence of the chemical potential,

$$\begin{aligned} \frac{dT'}{dZ} &< -\frac{Tg\beta}{C_p} + \frac{1}{\beta} \frac{1}{\rho} \frac{\delta \rho}{\delta c} \frac{dc}{dZ} \\ &= -1.4 \times 10^{-6} + 34.1 \frac{dc}{dZ} \end{aligned}$$

for water, where  $c$  is in % (g. of NaCl per 100g of  $H_2O$ ). The concentration gradient clearly dominates the stability:

- a) For a mean  $\bar{c} = 0.25\%$  and  $c$  varying linearly over the 12m height, convection will occur for

$$\frac{dT'}{dZ} < \pm 1.42 \text{ }^\circ\text{C/m.}$$

$\pm$  depending on the sign of the concentration gradient.

- b) For  $c$  varying linearly from 0 to 0.25% over the one week diffusion length of 24mm convection will occur in the diffusion region for

$$\frac{dT'}{dZ} < \pm 355 \text{ }^\circ\text{C/m.}$$

Landau and Lifshitz also provide conditions for the onset of convection in a fluid bounded by planes at  $Z = 0$  and  $Z = l$  with a temperature difference  $\Delta T$ , in terms of the Prandtl, Grashof, and Rayleigh numbers  $P$ ,  $G$  and  $Ra$  respectively.

$$P = \nu/\chi = 9.74 \text{ for } H_2O$$

$$G = \beta g l^3 \Delta T/\nu^2 \text{ and } Ra = GP,$$

where  $\chi = K/\rho C_p$  is the thermometric conductivity

$$V = \eta/\rho \text{ is the kinematic viscosity}$$

Steady convection must occur for  $GP > 1710$ , or 1100 for a free upper surface at  $T_1$ , and turbulent convection sets in  $G \geq 5 \times 10^4$ . For water and  $l = 10m$

$$G = 1.2 \times 10^{13} \Delta T/l$$

and a temperature gradient  $< -4 \times 10^{-9} \text{ }^\circ\text{C/m}$  is sufficient to induce turbulence. The conditions for the onset of convection apply for an incompressible fluid, but that is a good approximation for water.

## Appendix III

## Convection in SNO

Zwart and Van Doormaal (ASC Report 90-1022-1, Appendix B, Dec. 1990), estimate the scale magnitudes for the H<sub>2</sub>O as follows:

Heat transfer	10 + 2KW	(given)
Mass transfer	2.5 Kg s <sup>-1</sup>	(given)
Length scale	27m	(given)
Temperature difference	$\Delta T = 1^\circ\text{C}$	
Grashof number	$G = 10^{13}$	
Rayleigh number	$Ra = 10^{14}$	
Characteristic time	$\Delta t = 7 \text{ min}$	
Characteristic velocity	$v = 6 \text{ mm/s}$	

The convective time scale is given in the ASC report as

$$\Delta t = \frac{L^2}{\alpha} \sqrt{Ra^{-1}(1 + Pr^{-1})}$$

$$\sim \sqrt{1\nu / g\beta\chi\Delta T}$$

and the characteristic velocity as  $v = l/\Delta t$ .

Turbulent convection in the H<sub>2</sub>O is very probable (see however Section 0 of ASC report) and the ASC calculations indicate a temperature gradient in the H<sub>2</sub>O adjacent to the acrylic vessel of a few milli-degrees c per metre. Both positive and negative gradients are obtained in the various calculations although it is pointed out that a negative gradient, which would tend to drive convection in the D<sub>2</sub>O, is inherently unstable. If the gradient is negative, convection could occur transporting a few watts (limited by the thermal impedance of the acrylic) with a convective time scale of order of an hour, assuming of course that the recirculated D<sub>2</sub>O does not set up a temperature gradient. The Grashof number is large,  $\sim 10^{10}$ , so presumably the convection would be turbulent.

If the recirculated D<sub>2</sub>O were returned to the top of the acrylic vessel at -1°C relative to the bulk of the D<sub>2</sub>O, turbulent convection would be expected with a time scale of minutes, similar to the H<sub>2</sub>O. A positive concentration gradient of salt, resulting from returning the -1°C D<sub>2</sub>O with a relatively high concentration of salt, can only enhance the convective mixing.

The converse situation in which (pure) D<sub>2</sub>O is returned to the top of the acrylic vessel at +1°C relative to the bulk, has a positive temperature gradient and convection does not occur. This is a familiar situation in the laboratory and for that matter in any domestic hot water storage tank. If there is a negative concentration gradient that will also act against convection and should suppress convection even in the case of a negative temperature gradient of moderate magnitude.

It seems most unlikely that the H<sub>2</sub>O temperature gradient of a few milli-degrees per m acting via the considerable thermal impedance of the acrylic vessel can invalidate the conclusions drawn for D<sub>2</sub>O temperature gradients of  $\sim 100$  milli-degrees/m, or equivalent concentration gradients, set up by recirculation.