# A Condition for the Absence of Convection in Light and Heavy Water SNO-STR-95-051

S.J. Brice. Oxford University

November 23, 1995

**Abstract**

Conditions are derived which apply to the temperature and vertical temperature gradient and stipulate the circumstances under which $D_2O$ and $H_2O$ are mechanically stable. These conditions apply microscopically to any fluid element, but only restrict free convection.

## 1 Basis and Assumptions

This paper is a simple application of ideas in [LL59] with $D_2O$ and $H_2O$ data taken from [Kel67], [Kir51], and [KL86]. It assumes that the fluids are incompressible and in hydrostatic equilibrium. It further assumes that the specific heat capacity at constant pressure $C_p$ is constant over the temperature range of interest (5 - 40 °C) and that any convection is free, that is to say not driven by external forces such as fluid inflow or outflow. It should be noted that the following derivation produces a condition for the **absence** of convection. Violation of the condition does **not** imply the presence of convection. It this sense it is a necessary but not sufficient condition for mechanical stability.

## 2 The Derivation

Consider a fluid element at height $z$ and with density $\rho$. The state of this fluid element is specfied by any two thermodynamic quantities and so the density $\rho(p, s)$ can be expressed as a function of the equilibrium pressure $p$ and entropy $s$ at height $z$. If this element undergoes an adiabatic upward displacement through the small interval $\xi$ then its density becomes $\rho(p', s)$, where $p'$ is the pressure at its new position. For this equilibrium to be stable it is necessary (but not sufficient) that the forces on the element tend to return it to its original position i.e. for the element to be denser than the fluid it displaces. This displaced fluid will have density $\rho(p', s')$, where $s'$ is the equilibrium entropy at height $z + \xi$. The stability condition is therefore

$$\rho(p', s) > \rho(p', s') \tag{1}$$

Expanding $\rho(p', s')$ in powers of $(s' - s)$ gives

$$\rho(p', s') = \rho(p', s) + \left.\frac{\partial \rho}{\partial s}\right)_p (s' - s) + O[(s' - s)^2] \tag{2}$$

With $(s' - s) = \xi \frac{ds}{dz}$ and $\xi$ positive then the stability condition becomes

$$\left.\frac{\partial \rho}{\partial s}\right)_p \frac{ds}{dz} < 0 \tag{3}$$

Using the thermodynamic identity

$$\left.\frac{\partial \rho}{\partial s}\right)_p = \frac{T}{C_p} \left.\frac{\partial \rho}{\partial T}\right)_p \tag{4}$$

and noting that both $T$ and $C_p$ are positive enables Eqn. 3 to be written as

$$\left.\frac{\partial \rho}{\partial T}\right)_p \frac{ds}{dz} < 0 \tag{5}$$

The entropy gradient can also be transformed into a more friendly form

$$\frac{ds}{dz} = \left.\frac{\partial s}{\partial T}\right)_p \frac{dT}{dz} + \left.\frac{\partial s}{\partial p}\right)_T \frac{dp}{dz} \tag{6}$$

$$= \frac{C_p}{T}\frac{dT}{dz} + \frac{1}{\rho^2} \left.\frac{\partial \rho}{\partial T}\right)_p \frac{dp}{dz} \tag{7}$$

Putting this into Eqn. 5 yields

$$\frac{C_p}{T} \left.\frac{\partial \rho}{\partial T}\right)_p \frac{dT}{dz} < -\frac{1}{\rho^2} \left[ \left.\frac{\partial \rho}{\partial T}\right)_p \right]^2 \frac{dp}{dz} \tag{8}$$

With the assumption of hydrostatic equilibrium

$$\frac{dp}{dz} = -g\rho \tag{9}$$

and so

$$\left.\frac{\partial \rho}{\partial T}\right)_p \frac{dT}{dz} < \frac{g}{C_p}\frac{T}{\rho} \left[ \left.\frac{\partial \rho}{\partial T}\right)_p \right]^2 \tag{10}$$

Eqn. 10 is the condition for mechanical stability i.e. the condition that convection is absent.

## 3 The Application

The assumption of incompressibility ensures that $\rho$ and its temperature gradient are independent of pressure and can be considered as a function of temperature only. [Kel67] has an analytic expression for $\rho$ as a function of $T$ that applies to both light and heavy water and is accurate to $\sim$ 10 ppm over the relevant range of temperatures. This expression is

$$\rho(T) = \frac{a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 + a_5 T^5}{1 + b_1 T} \tag{11}$$

The relevant coefficients for light and heavy water are listed in Table 1.

Eqn. 11 means that $\rho$ and $\left.\frac{\partial \rho}{\partial T}\right)_p$ can be written analytically as functions of $T$. As previously noted $C_p$ can be assumed constant with temperature and its value for light and heavy water as well as the temperature where the densities are maximal are listed in Table 2

| | $a_0$ | $10^3 a_1$ | $10^6 a_2$ | $10^9 a_3$ | $10^{12} a_4$ | $10^{15} a_5$ | $10^3 b_1$ |
|---|---|---|---|---|---|---|---|
| $D_2O$ | 1.104690 | 20.09315 | -9.24227 | -55.9509 | 79.9512 | 0.0 | 17.96190 |
| $H_2O$ | 0.9998396 | 18.224944 | -7.922210 | -55.44846 | 149.7562 | -393.2952 | 18.159725 |

Table 1: The coefficients for Eqn. 11 giving $\rho$ in g cm$^{-3}$ as a function of $T$ in °C.

| | $C_p$ (J g$^{-1}$ K$^{-1}$) | $T_{\rho_{\max}}$ (°C) |
|---|---|---|
| $D_2O$ | 4.22 | 11.185 |
| $H_2O$ | 4.19 | 3.984 |

Table 2: The specific heat capacity and temperature of maximum density for light and heavy water

Given that

$$\begin{aligned} \left.\frac{\partial\rho}{\partial T}\right)_p &> 0 \qquad\qquad T < T_{\rho_{\max}} \\ \left.\frac{\partial\rho}{\partial T}\right)_p &< 0 \qquad\qquad T > T_{\rho_{\max}} \end{aligned} \tag{12}$$

then Eqn. 10 can be written as

$$\begin{aligned} \frac{dT}{dz} &< \frac{g}{C_p}\frac{T}{\rho}\left.\frac{\partial\rho}{\partial T}\right)_p \qquad\qquad T < T_{\rho_{\max}} \\ \frac{dT}{dz} &> \frac{g}{C_p}\frac{T}{\rho}\left.\frac{\partial\rho}{\partial T}\right)_p \qquad\qquad T > T_{\rho_{\max}} \end{aligned} \tag{13}$$

Using Eqns. 11 and 13 and the data of Tables 1 and 2 then Figs. 1 and 2 can be constructed. They show the regions of the $T - \frac{dT}{dz}$ plane for $D_2O$ and $H_2O$ respectively where convection cannot occur. Table 3 also lists the bounds of the non-convective region for various temperatures. For free convection, Figs. 1 and 2 can be used to indicate the mechanical stability of a particular location in the fluid.

# References


[Kel67] G. S. Kell. Precise representation of volume properties of water at one atmosphere. *Journal of Chemical and Engineering Data*, pages 66 – 69, 1967.

[Kir51] I. Kirshenbaum. *Physical Properties and Analysis of Heavy Water.* McGraw-Hill, 1951.

[KL86] G. W. C. Kaye and T. H. Laby. *Tables of Physical and Chemical Constants.* Longman Scientific and Technical, 1986.

[LL59] L. D. Landau and E. M. Lifshitz. *Fluid Mechanics.* Pergamon Press, 1959.

| $T$ (°C) | $D_2O$ $\frac{dT}{dz}$ range (°C $m^{-1}$) | $H_2O$ $\frac{dT}{dz}$ range (°C $m^{-1}$) |
|---|---|---|
| 2 | — | $< 0.0210$ |
| 4 | $< 0.0866$ | $> -0.000167$ |
| 6 | $< 0.0607$ | $> -0.0203$ |
| 8 | $< 0.0363$ | $> -0.0396$ |
| 10 | $< 0.0132$ | $> -0.0580$ |
| 12 | $> -0.00885$ | $> -0.0758$ |
| 14 | $> -0.0299$ | $> -0.0929$ |
| 16 | $> -0.0501$ | $> -0.110$ |
| 18 | $> -0.0695$ | $> -0.126$ |
| 20 | $> -0.0882$ | $> -0.141$ |

| $T$ (°C) | $D_2O$ $\frac{dT}{dz}$ range (°C $m^{-1}$) | $H_2O$ $\frac{dT}{dz}$ range (°C $m^{-1}$) |
|---|---|---|
| 22 | $> -0.106$ | $> -0.156$ |
| 24 | $> -0.124$ | $> -0.171$ |
| 26 | $> -0.141$ | $> -0.186$ |
| 28 | $> -0.157$ | $> -0.200$ |
| 30 | $> -0.174$ | $> -0.214$ |
| 32 | $> -0.189$ | $> -0.228$ |
| 34 | $> -0.205$ | $> -0.241$ |
| 36 | $> -0.220$ | $> -0.255$ |
| 38 | $> -0.235$ | $> -0.268$ |
| 40 | $> -0.250$ | $> -0.281$ |

Table 3: For various temperatures the range of $\frac{dT}{dz}$ where convection cannot occur.

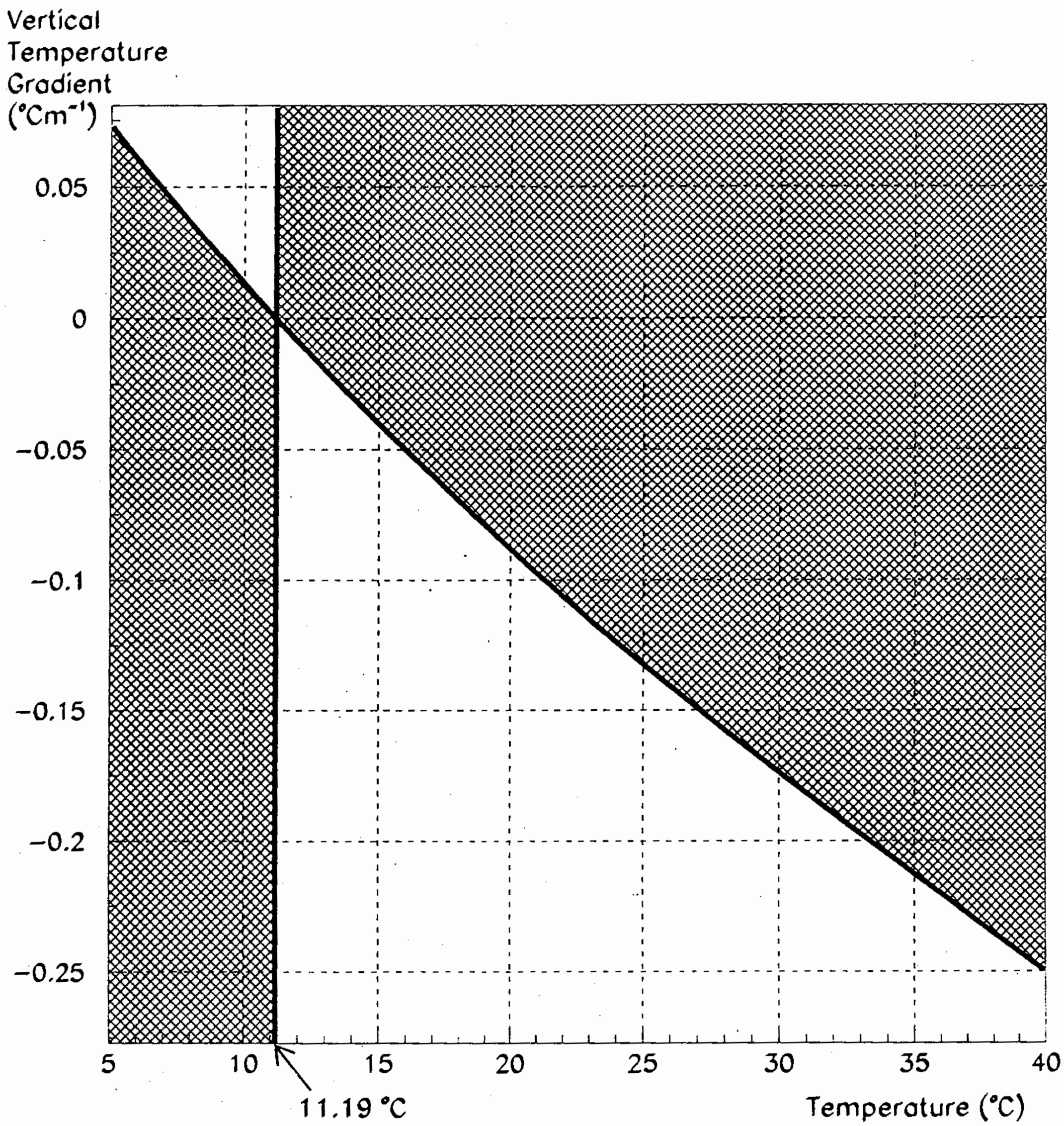


Figure 1: The shaded regions of the $T - \frac{dT}{dz}$ plane indicate where free convection in $D_2O$ cannot occur.

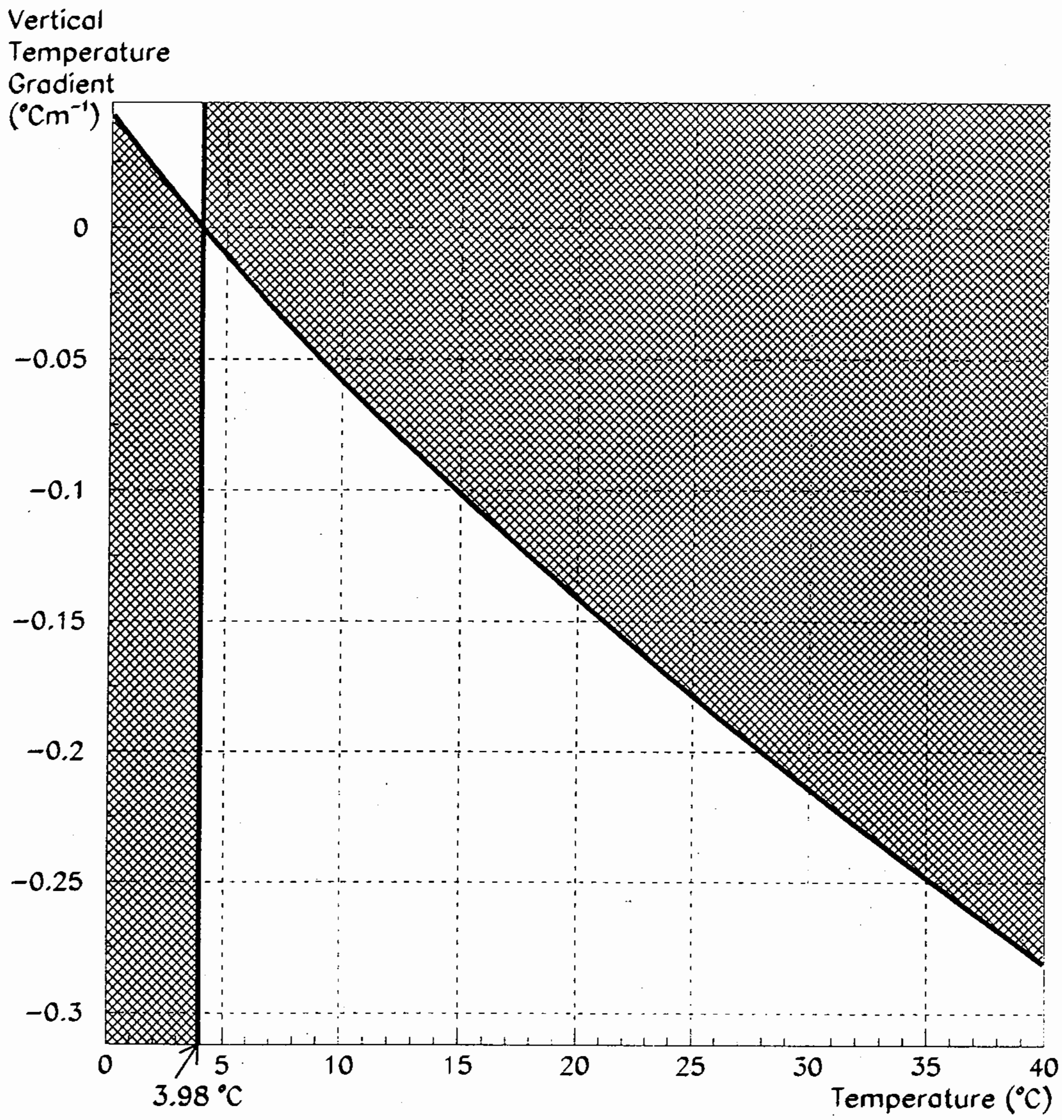


Figure 2: The shaded regions of the $T - \frac{dT}{dz}$ plane indicate where free convection in $H_2O$ cannot occur.