Scoping Calculations for Natural Convection

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Introduction

The goal is to demonstrate the feasibility of cooling a molten salt fuel tube via natural convection, allowing the complete elimination of pumps from the system. First it is necessary to consider the heat transfer coefficient in from the fuel tube wall to the coolant. First we review the models for a vertical plate (which are readily extended to a cylinder). Then, we derive the temperature profile in the rod (assuming only conductive heat transfer) for an arbitrary volumetric heat generation rate $\dot{q}_{\text{gen}}$. Finally, using a representative salt composition, the thermophysical properties may be evaluated (using the MSTDB) and the rod centerline temperature can be calculated as a function of $\dot{q}_{\text{gen}}$.

Free Convection on a Vertical Surface

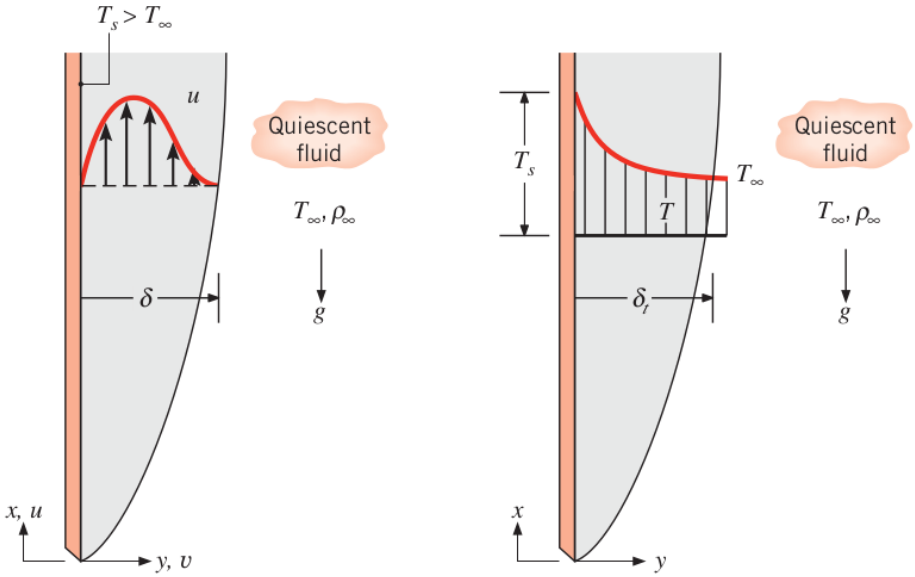

Figure 1: Boundary layer development on a hot vertical plate. Velocity boundary layer (left), thermal boundary layer (right). Taken from [2]

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Considering a laminar boundary layer flow driven by buoyancy forces alone (shown in Fig. 1) and steady, two dimensional, constant property conditions in which gravity acts in the $-x$ direction. Further, we assume the fluid is *incompressible* except for accounting for the density variation in the buoyancy force as it is the primary driving force of the flow (the validity of assuming incompressibility with respect to all other terms is discussed in [6]). Further, we assume the classical boundary layer approximations are valid (section 6.4.1

of [2]), namely that the pressure gradient within the boundary layer can be approximated by the free-stream pressure gradient, i.e.

$$\frac{\partial p}{\partial x} \approx \frac{dp_\infty}{dx}$$

which in this case is just $-\rho_\infty g$ (the hydrostatic pressure gradient). This is usually a good approximation because the boundary layer is so thin. These assumptions allow us to derive the boundary layer equations (with a body force)

$$\begin{aligned} u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} &= -\frac{1}{\rho}\frac{dp_\infty}{dx} - g + \nu\frac{\partial^2 u}{\partial y^2} \\ &= \frac{\rho_\infty g}{\rho} - g + \nu\frac{\partial^2 u}{\partial y^2} \\ &= g\frac{\rho_\infty - \rho}{\rho} + \nu\frac{\partial^2 u}{\partial y^2} \equiv g\frac{\Delta\rho}{\rho} + \nu\frac{\partial^2 u}{\partial y^2} \end{aligned}$$

the first term on the right hand side of the above equation is the buoyance force per unit mass, and is the driver for natural convection. If the density variations are due *only* to temperature vaariations, the buoyancy term may be related to a fluid property called the *volumentric thermal expansion coefficient* [2], defined as

$$\beta = -\frac{1}{\rho}\left(\frac{\partial\rho}{\partial T}\right)_p$$

which measures the reponse of density to a temperature variation at constant pressure. This term can be approximated as

$$\begin{aligned} \beta &\approx -\frac{1}{\rho}\frac{\Delta\rho}{\Delta T} = -\frac{1}{\rho}\frac{\rho_\infty - \rho}{T_\infty - T} \\ \implies \rho_\infty - \rho &\approx \rho\beta\left(T - T_\infty\right) \end{aligned}$$

this is known as the *Boussinesq approximation* [2], which then allows us to express the buoyancy term solely in terms of the free stream temperature difference and the volumetric expansion coefficient (taken as a known fluid property), yielding

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = g\beta\left(T - T_\infty\right) + \nu\frac{\partial^2 u}{\partial y^2}$$

The buoyancy term effects only the momentum equation, and the energy and continuity equations take the usual form

$$\begin{aligned} \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} &= 0 \\ u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} &= \alpha\frac{\partial^2 T}{\partial y^2} \end{aligned}$$

note that the viscous dissipation term has been neglected in the energy equation, and is typically a good approximation for the low-velocity flows associated with natural convection [2]. Unfortunately, the buoyancy term introduces a critical dependence on temperature in the momentum equation, making it impossible for all of the equations to be decoupled (as is done for forced convection). Now, it's important to introduce the relevant dimensionless parameters

$$\begin{aligned} x^* = \frac{x}{L} \qquad y^* = \frac{y}{L} \\ u^* = \frac{u}{u_0} \qquad v^* = \frac{v}{u_0} \qquad T^* = \frac{T - T_\infty}{T_s - T_\infty} \end{aligned}$$

where L and u_0 are respective characteristic lengths and velocities for the flow. In terms of these dimensionless parameters, the x-momentum and energy equations reduce to

$$u^*\frac{\partial u^*}{\partial x^*} + v^*\frac{\partial u^*}{\partial y^*} = \frac{g\beta\left(T_s - T_\infty\right)L}{u_0^2}T^* + \frac{1}{\mathrm{Re}_L}\frac{\partial^2 u^*}{\partial y^{*2}}$$
$$u^*\frac{\partial T^*}{\partial x^*} + v^*\frac{\partial T^*}{\partial y^*} = \frac{1}{\mathrm{Re}_L\mathrm{Pr}}\frac{\partial^2 T^*}{\partial y^{*2}}$$

It's convenient to define the (as of yet) arbitrary reference velocity u_0 so that the term multiplying T^* in the first equation is unity, this requires

$$u_0^2 = g\beta\left(T_s - T_\infty\right)L$$

which also effects the Reynolds number (because it explicitly involves the reference velocity), making it

$$\mathrm{Re}_L = \left[\frac{g\beta\left(T_s - T_\infty\right)L^3}{\nu^2}\right]^{1/2}$$

it's then customary to define the *Grashof number* Gr_L as the square of this Reynolds number

$$\mathrm{Gr}_L \equiv \frac{g\beta\left(T_s - T_\infty\right)L^3}{\nu^2}$$

This dimensionless number is a ratio of bouyancy forces to viscous forces (rather than inertial to viscous as was the case for the Reynolds number in the nonbouyant case). In addition, it's useful to define the Rayleigh number

$$\mathrm{Ra}_L = \mathrm{Gr}_L\mathrm{Pr} = \frac{g\beta\left(T_s - T_\infty\right)L^3}{\nu\alpha}$$

Where the Prandtl number is given by

$$\mathrm{Pr} = \frac{\alpha}{\nu} = \frac{\nu}{k/\left(\rho c_p\right)}$$

and is the ratio between thermal and viscous diffusivity.

The Correlations

For the case of laminar flow ($\mathrm{Ra_L} \leq 10^9$) the correlation for the surface averaged Nusselt number is given by

$$\overline{\mathrm{Nu}}_L = \frac{\overline{h}L}{k} = \frac{4}{3}\left(\frac{\mathrm{Gr}_L}{4}\right)^{1/4} g\left(\mathrm{Pr}\right)$$
$$g\left(\mathrm{Pr}\right) = \frac{0.75\mathrm{Pr}^{1/2}}{\left(0.609 + 1.221\mathrm{Pr}^{1/2} + 1.238\mathrm{Pr}\right)^{1/4}}$$

For non laminar flows, the correlations suitable for many engineering calculations are often of the form

$$\overline{Nu}_L = \frac{\overline{h}L}{k} = C\mathrm{Ra}_L^n$$

for laminar flow with $10^4 \leq \mathrm{Ra}_L \leq 10^9$, $C = 0.59$ and $n = 1/4$, for combined laminar and turbulent flow ($10^9 \leq \mathrm{Ra}_L \leq 10^{13}$), $C = 0.1$ and $n = 1/3$. Alternatively, a correlation that may be used over the *entire* range of Ra_L has been suggested [2] and has the form

$$\overline{Nu}_L = \left[0.825 + \frac{0.387\mathrm{Ra}_L^{1/6}}{\left[1 + \left(0.492/\mathrm{Pr}\right)^{9/16}\right]^{8/27}}\right]^2$$

where L is the plate length. Slightly better accuracy may be obtained for laminar flow by using

$$\overline{Nu}_L = 0.68 + \frac{0.670\mathrm{Ra}_L^{1/4}}{[1+(0.492/\mathrm{Pr})^{9/16}]^{4/9}} \qquad \mathrm{Ra}_L \leq 10^9$$

Critically, the above results may be applied to vertical *cylinders* of height L if the boundary layer thickness δ is much less than the cylinder diameter D. This condition is known to be satisfied when [2]

$$\frac{D}{L} \geq \frac{35}{\mathrm{Gr}_L^{1/4}} \tag{1}$$

slender cylinders where transverse curvature influences the boundary layer development actually have enhanced heat transfer. Correlations have been provided in the literature for these cases as well.

The Inter-Pin Radial Temperature Profile

Assuming only conduction, the radial temperature profile for a solid sphere with an arbitrary volumetric heat generation rate $\dot{q}_{\mathrm{gen}}$, surface temperature T_s, and outer radius r_o is given by (Section 3.5.2 of [2])

$$T(r) = \frac{\dot{q}r_o^2}{4k}\left(1 - \frac{r^2}{r_o}\right) + T_s$$

We may also relate the surface temperature to the temperature of the cold (coolant molten salt) by performing an energy balance on the outer surface, which gives

$$T_s = T_\infty + \frac{\dot{q}r_o}{2h}$$

Note that the centerline temperature (which will be design limiting in our case) is given by

$$T(0) = \frac{\dot{q}r_o^2}{4k} + T_\infty + \frac{\dot{q}r_o}{2h}$$

Choice of a Reference Salt

We use the same salt compositions as [4] being that it is the only other fast-spectrum reactor concept using the same fuel tube design that has been published. That is, the fuel salt has the following composition NaCl-$PuCl_3$-UCl_3 (60-20-20 mol%), and the coolant salt has the composition ZrF_4-NaF-KF (42-10-48 mol%). However, this exact composition is not available in the molten salt thermal properties database. This can be mitigated by using the Redlich-Kister to expand the (temperature varying) properties as a function of composition (mol fraction of end members) as detailed in [1], but for an initial simplistic analysis, we can just alter the composition to coincide with that in the database i.e. ZrF_4-NaF-KF (52-5-52 mol%) which is close enough to the Moltex reference in any case. Unfortunately, the Molten Salt Thermal Properties Database (MSTDB [7]) is currently lacking almost all ternary chloride systems, so we will instead perform a *crude* approximation by taking the properties of the ternary system to be the average of those for the individual binary systems (i.e. $\mathrm{NaCl} - \mathrm{PuCl_3}$ (75-25 mol%) and $\mathrm{NaCl} - \mathrm{UCl_3}$ (75-25 mol%)). First note that in the MSTDB, density is intepolated via

$$\rho = A - BT$$

The exact composition (i.e. (75-25 mol%)) was available for the Pu binary system, which gives density coefficients In this case, since we have an analytical expression for the temperature variation of the density so we can analytically compute β in terms of A and B (assuming these values were taken at constant pressure). By definition

$$\begin{aligned}\beta &= -\frac{1}{\beta}\left(\frac{\partial\rho}{\partial T}\right)_p \\ &= -\frac{1}{A-BT}(-B) \\ &= \frac{B}{A-BT}\end{aligned}$$

	A (kg/m^3)	B ($\frac{kg}{m^3 \cdot K}$)
NaCl-$PuCl_3$ (75-25 mol%)	3630	0.846
NaCl-UCl_3 (71.7-28.4 mol%)	3850	0.885
Estimated NaCl-$PuCl_3$-UCl_3 (60-20-20 mol%)	3740	0.8655
ZrF_4-NaF-KF (52-5-52 mol%)	3380	0.84

Table 1: Density expansion coefficients for salt components

The remaining values were not available in the database, and may result in *large* errors, but for the sake of concreteness, we choose constant thermal conductivities of 0.5W/mK and 0.7W/mK and melting points of 738 K and 698 K for the fuel and coolant salt respectively (as used in Chapter 14 of [4]). Additionally, we take the fuel salt boiling point to be 1837 K (as in Chapter 14 of [4]).

The Prandtl Number

Finally, to evaluate the Prandtl number (only needed for the coolant, since we're considering free convection of the coolant only) we need the viscosity and heat capacity. In the MSTDB viscosity is parameterized as

$$\nu = A \exp\left(\frac{B}{RT}\right)$$

where R is the ideal gas constant ($R = 8.314 J/K$), and the viscosity is given in units of $\frac{mN \cdot s}{m^2}$ and so must be multiplied by 10^{-3} in all applications. For the coolant salt, it was found that $A = 0.161$ and $B = 26400$. Unfortunately, no heat capacity data was supplied for the chosen coolant salt, and so a crude estimate had to be employed. In Chapter 14 of [4], the author states that the heat capacity varies between 510 and 700 $\frac{J}{kg \cdot K}$ over the temperature range of 500-1500 °C. This variation was fit to a linear model of the form

$$c_p = A + BT$$

from which it was calculated that $A = 363.1 \frac{J}{kg \cdot K}$ and $B = 0.19 \frac{J}{kg \cdot K^2}$.

The Calculation

For the calculation, a heated rod height of $L = 2.6m$ was used (taken from the relevant chapter discussing Moltex's previous design: the SSRU [5]). Additionally it was assumed that the coolant salt inlet temperature is 100 K over the evaluated melting temperature (i.e $T_\infty = 838$ K). Notably, there are still the heat generation rate and the fuel pin radius r_o that have yet to be chosen. To explore the design space, these quantities were taken to be variable, and the fuel centerline temperature was calculated as a function of these. The chosen range was $r_o \in [2 - 10]mm$ and $\dot{q} \in [0, 200] kW/L$ noting that a typical LWR has $r_o = 4.5mm$ and $\dot{q} = 100 kW/L$.

Iterative Calculation of Rayleigh Number

The only thing left to note is that the Rayleigh number (which needs to be calculated to evaluate the Nusselt number and the subsequent heat transfer coefficient) depends on the surface temmperature, which is itself a function of the heat transfer coefficient. Additionally, it is customary to evaluate coolant properties at the average temperature $T_{eval} = \frac{1}{2}(T_\infty + T_s)$, so an iterative calculation on the heat transfer coefficient and surface temperature must be performed. In practice, this is performed by iteratively updating the heat transfer coefficient and surface temperature. By performing sensitivity on the number of iterations, it was determined that 100 inner iterations (to converge h and T_s) was adequate (i.e. resulting in no noticable change in the final results). The python implementation is shown below

```
# Need two loops, one over volumetric  heat generation rate (in W/m3) and one for fuel pin
                                        radius ro
qgens = np.linspace(0, 200E+06, 100) # W/m3
```

```
ros = np.linspace(0.002, 0.01, 5) # 2mm-10mm

for ro in ros:
    centerlineTemps = np.zeros(len(qgens))
    for index, qgen in enumerate(qgens):
        hguess = 1 # initial guess of h
        Tsguess = 500 # initial guess of surface temp
        for i in range(100):
            Teval = 1/2*(Tsguess + Tinf) # Properties evaluated at average temp
            Nu = NuL(Teval, hguess, qgen, ro)
            hguess = kc/L*Nu # Update guess of h
            Tsguess = Ts(hguess, qgen, ro)
        centerlineTemps[index] = centerlineTemp(Tsguess, qgen, ro)
```

Validity

On each outer iteration (over $\dot{q}$ and r_o) the condition for using the vertical plate correlation (Eq. 1) was evaluated, and not a single iteration did not satisfy the condition (due to the relatively large L).

Results

The results are shown in Fig. 2. As compared with an LWR, a much smaller pin radius is needed (around twice as small) to achieve similar power densities while maintaining a reasonable 200 K boiling margin (a 800 pcm reactivity insertion results in a 120 °C temperature increase [3], so 200 K is conservative) which is to be expected because of the poor thermal conductivity of molten salts. What is important is that this calculation demonstrates the feasability of using *natural convection* to cool the reactor, allowing the complete elimination of pumps from the design, which represent both a safety hazard and a large technical challenge for conventional molten salt reactors.

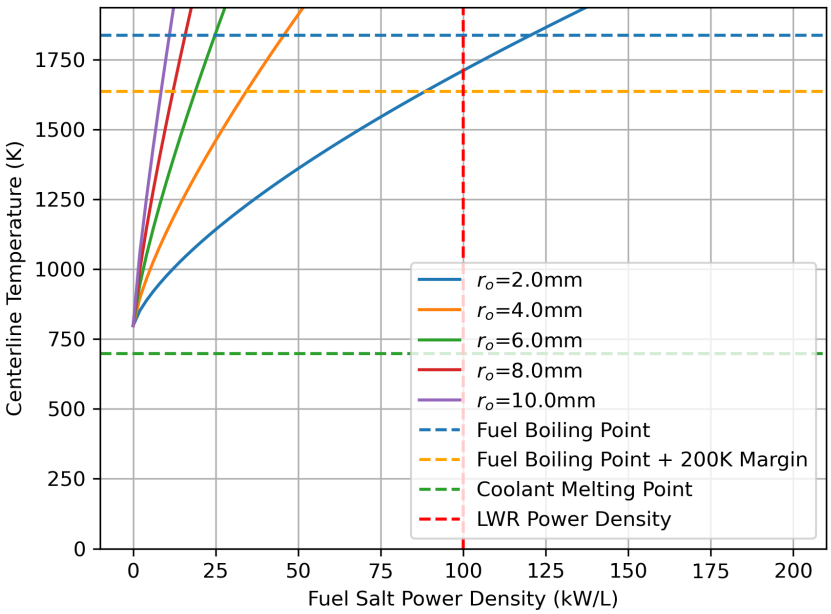

Figure 2: Fuel centerline temperature as a function of volumetric heat generation ($\dot{q}$) and rod outer radius (r_o)

References

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[3] Mazen Bushnaga, Taesuk Oha, and Yonghee Kima. "A Neutronic Study on Safety Characteristics of Fast Spectrum Stable Salt Reactor (SSR)". In: (2021).

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[7] Nick Termini et al. "An Overview of the Molten Salt Thermal Properties Database–Thermophysical, Version 2.1.1 (MSTDB-TP v.2.1.1)". In: (July 2023). DOI: 10.2172/1988348. URL: https://www.osti.gov/biblio/1988348.