Diffusion equation in multiplying medium: the Buckling Equation

Steady state multi energy group neutron diffusion equation for multiplying medium can be given by,

$$-\vec{\nabla}\cdot(D_g(\vec{r})\,\vec{\nabla}\Phi_g(\vec{r}))+\Sigma_{rem}^{g}(\vec{r})\Phi_g(\vec{r})=\chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}(\vec{r})\Phi_{g'}(\vec{r})+\sum_{\substack{g'=1\\ g'\neq g}}^{G}\Sigma_{scat}^{g'\to g}(\vec{r})\Phi_{g'}(\vec{r})$$

In this expression, the neutron population balance and Fick's law are combined together.

For the simplest case where the cross-sections doesn't depend on position, the equation reduces to,

$$-D_g\nabla^2\Phi_g(\vec{r})+\Sigma_{rem}^{g}\Phi_g(\vec{r})=\chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\Phi_{g'}(\vec{r})+\sum_{\substack{g'=1\\ g'\neq g}}^{G}\Sigma_{scat}^{g'\to g}\Phi_{g'}(\vec{r})$$

If the space and energy dependency is assumed to be separable. Let,

$$\Phi_g(\vec{r})=\psi(\vec{r})\phi_g$$

In such a case, the above diffusion equation becomes,

$$-D_g\phi_g\nabla^2\psi(\vec{r})+\Sigma_{rem}^{g}\phi_g\psi(\vec{r})=\chi_g\psi(\vec{r})\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'}+\psi(\vec{r})\sum_{\substack{g'=1\\ g'\neq g}}^{G}\Sigma_{scat}^{g'\to g}\phi_{g'}$$

$$\implies -D_g\phi_g\nabla^2\psi(\vec{r})=\chi_g\psi(\vec{r})\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'}+\psi(\vec{r})\sum_{\substack{g'=1\\ g'\neq g}}^{G}\Sigma_{scat}^{g'\to g}\phi_{g'}-\Sigma_{rem}^{g}\phi_g\psi(\vec{r})$$

$$\implies -\frac{\nabla^2\psi(\vec{r})}{\psi(\vec{r})}=\frac{\chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'}+\sum_{\substack{g'=1\\ g'\neq g}}^{G}\Sigma_{scat}^{g'\to g}\phi_{g'}-\Sigma_{rem}^{g}\phi_g}{D_g\phi_g}$$

Since the spatial part and energy dependent part are completely separated, both should be equal to some constant.

$$-\frac{\nabla^2\psi(\vec{r})}{\psi(\vec{r})}=\frac{\chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'}+\sum_{\substack{g'=1\\ g'\neq g}}^{G}\Sigma_{scat}^{g'\to g}\phi_{g'}-\Sigma_{rem}^{g}\phi_g}{D_g\phi_g}=B^2$$

Why B^2 is chosen as the constant, why not $-B^2$?

For a critical system, the neutron number will be balanced by neutron source, absorption and leakage. The source will be more so that the neutron leakage is positive. The energy dependent second term clearly shows that numerator is fission source+scattering source-removal of neutrons from the group, which is bound to be positive for a critical system. At the same time, diffusion equation is also always positive (inverse to transport cross-section, which is a positive quantity). This is the reason why B^2 is chosen as the constant.
In short, this choice ensures that we get a positive leakage term which is expected in a critical system.

This gives two equations, first equation entirely depends on space and hence the corresponding constant is called geometrical buckling,

$$\nabla^2\psi + B_g^2\psi = 0$$

The second equation is entirely depend on multi energy group neutron reaction cross-section and corresponding constant is called material buckling,

$$(B_m^2 D_g + \Sigma_{rem}^g)\phi_g = \chi_g \sum_{g'=1}^{G} \nu\Sigma_f^{g'}\phi_{g'} + \sum_{\substack{g'=1 \\ g' \neq g}}^{G} \Sigma_{scat}^{g'\to g}\phi_{g'}$$

Relation between geometrical and material buckling

For a critical system, the geometrical and material buckling are equal,

$B_g^2 = B_m^2 \implies$ critical system; k=1; $\Phi_g(\vec{r}, t)$ will not change with time

But in general, this is not true. For a general system, the diffusion equation will be,

$$-\overrightarrow{\nabla}\cdot(D_g(\vec{r})\overrightarrow{\nabla}\Phi_g(\vec{r}) + \Sigma_{rem}^g(\vec{r})\Phi_g(\vec{r}) = \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_f^{g'}(\vec{r})\Phi_{g'}(\vec{r}) + \sum_{\substack{g'=1 \\ g' \neq g}}^{G}\Sigma_{scat}^{g'\to g}(\vec{r})\Phi_{g'}(\vec{r})$$

Performing the similar analysis as above, this equation gives

$$-\frac{\nabla^2\psi(\vec{r})}{\psi(\vec{r})} = \frac{\frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'} + \sum_{\substack{g'=1 \\ g' \neq g}}^{G}\Sigma_{scat}^{g'\to g}\phi_{g'} - \Sigma_{rem}^g\phi_g}{D_g\phi_g}$$

$$\implies -\frac{\nabla^2\psi(\vec{r})}{\psi(\vec{r})} = \frac{\frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'} - \chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'} + \chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'} + \sum_{\substack{g'=1 \\ g' \neq g}}^{G}\Sigma_{scat}^{g'\to g}\phi_{g'} - \Sigma_{rem}^g\phi_g}{D_g\phi_g}$$

$$\implies -\frac{\nabla^2\psi(\vec{r})}{\psi(\vec{r})} = \frac{\frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'} - \chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'}}{D_g\phi_g} + \frac{\chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'} + \sum_{\substack{g'=1 \\ g' \neq g}}^{G}\Sigma_{scat}^{g'\to g}\phi_{g'} - \Sigma_{rem}^g\phi_g}{D_g\phi_g}$$

Now, by the definition of geometrical buckling and material buckling this reduces to,

$$B_g^2 = \frac{\frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'} - \chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'}}{D_g\phi_g} + B_m^2$$

$$\implies B_m^2 - B_g^2 = \frac{\chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'} - \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'}}{D_g\phi_g}$$

$$\implies B_m^2 - B_g^2 = \frac{k_{eff}-1}{k_{eff}} \times \frac{\chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'}}{D_g\phi_g} = \rho \times \frac{\chi_g\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi_{g'}}{D_g\phi_g}$$

Where, ρ is the reactivity.

Both the terms $\chi_g \sum_{g'=1}^{G} \nu\Sigma_f^{g'}\phi_{g'}$ and $D_g\phi_g$ are non negative. Hence, the following can be concluded-

$B_m^2 > B_g^2 \implies \rho > 0; k_{eff} > 1; \Phi$ will increase with time
$B_m^2 = B_g^2 \implies \rho = 0; k_{eff} = 1; \Phi$ doesn't change with time
$B_m^2 < B_g^2 \implies \rho < 0; k_{eff} < 1; \Phi$ will decrease with time

Physical significance of B_g^2 will be described in later notes.

Solution of Geometrical Buckling equation in cylindrical geometry

Consider a fissile material in a cylinder surrounded by vacuum. The vacuum boundary condition, i.e. no incoming current condition can then be substituted by zero flux boundary condition by suitably increasing the radius and length of the cylinder by required amount. Let the extrapolated radius be R and length be L.
Hence the buckling equation becomes,

$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi(r,z)}{\partial r}\right) + \frac{\partial^2\psi(r,z)}{\partial z^2} + B_g^2\psi(r,z) = 0$ in the domain $\Omega : (0,R) \times \left(-\frac{L}{2},\frac{L}{2}\right)$

With B.C:

$$\psi(R,z) = 0, \forall z \in \left(-\frac{L}{2},\frac{L}{2}\right)$$

$$\psi\left(r, \pm\frac{L}{2}\right) = 0, \forall r \in (0,R)$$

Separation of variable method can be employed to solve the equation:

$\psi(r,z) = \xi(r)Z(z)$

By using this, the buckling equation becomes,

$$\frac{1}{r\xi(r)}\frac{d}{dr}\left(r\frac{d\xi(r)}{dr}\right) + \frac{1}{Z}\frac{d^2Z(z)}{dz^2} + B_g^2 = 0$$

Two separate equations are formed of this equation:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\xi(r)}{dr}\right) + B_r^2\xi(r) = 0$$

$$\frac{d^2Z(z)}{dz^2} + B_z^2 Z = 0$$

Where, $B_g^2 = B_r^2 + B_z^2$

Axial Part Solution:

Solution of the second equation is, $Z(z) \sim A\cos(B_z z) + B\sin(B_z z)$

If the boundary condition is is applied, $Z\left(\pm\frac{L}{2}\right) = 0$

Then a set of solutions are obtained,

$$Z(z) = \sum_{n=0}^{\infty} A_n \cos\left(\frac{(2n+1)\pi z}{L}\right) + B_n \sin\left(\frac{2n\pi z}{L}\right)$$

In general, these solution holds good with the condition $Z\left(-\frac{L}{2} \leq z \leq \frac{L}{2}\right) > 0$

because finally this should give neutron total flux, which should be non negative at all points in space (otherwise the reaction rates, i.e. number of reactions would become negative with is unfeasible).

The simplest solution with this condition is,

$Z(z) \sim \cos\left(\frac{\pi z}{L}\right)$ and $B_z = \frac{\pi}{L}$

In general case, coefficient of this term A_0 would dominate and coefficient of other terms $(A_1, B_1, A_2, B_2, \ldots)$ will be small,. Physically other terms can be thought of as disturbance over the dominating cosine term.

<u>Radial Part Solution:</u>

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\xi(r)}{dr}\right) + B_r^2\xi(r) = 0$$

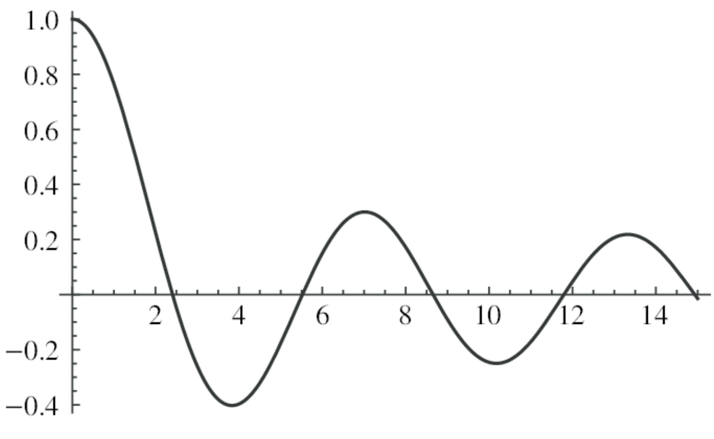
$$\implies \frac{d^2\xi(r)}{dr^2} + \frac{1}{r}\frac{d\xi(r)}{dr} + B_r^2\xi(r) = 0$$

$$\implies r^2\frac{d^2\xi(r)}{dr^2} + r\frac{d\xi(r)}{dr} + r^2B_r^2\xi(r) = 0$$

Substitute $x = rB_r$ gives,

$$\implies x^2\frac{d^2\xi(x)}{dx^2} + x\frac{d\xi(x)}{dx} + x^2\xi(x) = 0$$

This is Bessel's differential equation of order 0. The solution is, $\xi(x) = J_0(x) \implies \xi(r) = J_0(B_r r)$



The boundary condition is, $\xi(R) = 0 \implies J_0(B_r R) = 0.$

The zeros of the Bessel function occur at 2.4048, 5.5201, 8.6537, 11.7915, 14.9309,…
Hence the solution can be written as,

$\xi(r) = \sum_{n=1}^{\infty} C_n J_0\left(\frac{\nu_n r}{R}\right)$ where ν_n is the value where n-th zero of Bessel's function occur.

Since the flux has to be non negative at all points, in general the C_1 would dominate and all other terms will be as disturbance over the dominating term. Hence the simplest solution would be,

$\xi(r) \sim J_0\left(\frac{2.4048r}{R}\right)$ and $B_r = \frac{2.4048}{R}$

Total Solution:
All terms collected together,

$$\psi(r,z) = \psi_0 J_0\left(\frac{2.4048r}{R}\right)\cos\left(\frac{\pi z}{L}\right)$$

And $B_g^2 = B_r^2 + B_z^2 = \left(\frac{2.4048}{R}\right)^2 + \left(\frac{\pi}{L}\right)^2$

The constant ψ_0 is different for different energy groups. For simple 1-group diffusion equation, where $\psi(\vec{r}) = \Phi(\vec{r})$, the constant can be easily determined from the power of the reactor.

$$P = 2\pi\psi_0 w_f \Sigma_f \int_{r=0}^{R}\int_{z=-\frac{L}{2}}^{\frac{L}{2}} J_0\left(\frac{2.4048r}{R}\right)\cos\left(\frac{\pi z}{L}\right) rdrdz$$

Where, w_f = energy released in a fission

Note:
1. In multiplying medium, diffusion equation reduces to buckling equation
2. Unlike the case in of non-multiplying medium where a unique solution is obtained from diffusion equation, infinitely many solutions can be obtained in multiplying medium
3. Solution of buckling equation gives the shape of the flux, no absolute value of flux is obtained from this equation. This is because, the buckling equation in principle is a eigenvalue equation.
4. Physically this means that the reactor can be operated at any absolute flux, maintaining the flux shape. With increase in flux, the power of the reactor will also increase.
5. For infinite cylinder, $R \to \infty$ and $L \to \infty$ and in such a case, there will be no leakage from the system. The corresponding buckling $B_g^2 \to 0$. Hence, B_g^2 is a measure of neutron leakage from the system. Smaller is the core, higher the value of B_g^2 would be and there will be more leakage.

Relation between k_∞ and k_{eff}:

For the case where the material is extended to infinity, there will be no leakage from the system. The corresponding 1-group diffusion equation is given by,

$$\Sigma_a \Phi = \frac{\nu\Sigma_f\Phi}{k_\infty}$$

If, instead a finite amount of material is put, there would be leakage from the system. The corresponding 1 group diffusion equation is given by,

$$-D\nabla^2\Phi + \Sigma_a\Phi = \frac{\nu\Sigma_f\Phi}{k_{eff}}$$

k_∞ is clearly a material property and is called infinite multiplication factor. k_{eff} is called effective multiplication factor which takes the leakage into account due to finite nature of the system. Due to the buckling equation, it is possible to establish a relation between these two multiplication factor. For that, replace $D = L^2\Sigma_a$ and $\nabla^2\Phi = -B_g^2\Phi$ which is true for 1group system.

Then,

$$-D\nabla^2\Phi + \Sigma_a\Phi = \frac{\nu\Sigma_f\Phi}{k_{eff}}$$

$$\implies -L^2\Sigma_a(-B_g^2\Phi) + \Sigma_a\Phi = \frac{\nu\Sigma_f\Phi}{k_{eff}}$$

$$\implies (1 + B_g^2L^2)\Sigma_a\Phi = \frac{\nu\Sigma_f\Phi}{k_{eff}}$$

$$\implies k_{eff} = \frac{\frac{\nu\Sigma_f\Phi}{\Sigma_a\Phi}}{1 + B_g^2L^2} = \frac{k_\infty}{1 + B_g^2L^2}$$

This is again proves that for if B_g^2 increases, k_{eff} reduces. To get maximum k_{eff} from a system with given material, the B_g^2 should be as low as possible.

Minimum leakage condition in a cylindrical system of constant volume surrounded by vacuum:

To get minimum leakage, B_g^2 should be minimum. Since the volume $V = \pi R^2 L$ is constant, the leakage can be written in terms of only one parameter of the cylinder.

$$B_g^2 = \left(\frac{2.405}{R}\right)^2 + \left(\frac{\pi}{L}\right)^2 = \frac{2.405^2}{V}\pi L + \left(\frac{\pi}{L}\right)^2$$

Minimization condition:

$$\frac{dB_g^2}{dz} = 0$$

$$\implies \frac{2.405^2\pi}{V} - \frac{2\pi^2}{L^3} = 0$$

$$\implies \frac{2.405^2}{\pi R^2 L} - \frac{2\pi}{L^3} = 0$$

$$\implies \frac{2.405^2}{R^2} = \frac{2\pi^2}{L^2}$$

$$\implies \frac{L}{R} = \frac{\sqrt{2}\pi}{2.405} \approx 1.85$$

This result is sometimes loosely told as, the minimum leakage is possible when the cylinder length and diameter are almost equal.