RAPTOR equation summary

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1 Definitions & useful equations

RAPTOR uses right-handed (R, ϕ, Z) coordinate system and COCOS=11 with $\sigma_{I_p} = \sigma_{B_0} = 1$, since I_p and B_0 are always assumed positive [5].
Furthermore:
$\rho = \sqrt{\Phi/\pi B_0}, \quad \rho_b = \sqrt{\Phi_b/\pi B_0}, \quad \hat{\rho} = \sqrt{\Phi/\Phi_b}$
$V'_\rho = \frac{\partial V}{\partial \rho}$, $V'_{\hat{\rho}} = \frac{\partial V}{\partial \hat{\rho}}$
$g_0 = \langle \nabla V \rangle$, $g_1 = \left\langle (\nabla V)^2 \right\rangle$, $g_2 = \left\langle \frac{(\nabla V)^2}{R^2} \right\rangle$, $g_3 = \left\langle \frac{1}{R^2} \right\rangle$.
$F = RB_\phi$
$j_{ni} = \frac{\langle \mathbf{j_{ni}} \cdot \mathbf{B} \rangle}{B_0}$

From the chain rule, we can write the useful relation, for a quantity $A = A(t, \psi(\Phi))$

$$\left.\frac{\partial}{\partial t}\right|_\psi A(t,\psi) = \left.\frac{\partial A(\Phi,t)}{\partial t}\right|_\Phi + \left.\frac{\partial A(\Phi,t)}{\partial \Phi}\right|_t \left.\frac{\partial \Phi}{\partial t}\right|_\psi \tag{1}$$

2 Flux transport

Flux surface averaged ohm's law in general form:

$$\sigma_\parallel \left.\frac{\partial \Phi}{\partial t}\right|_\psi = \frac{F^2}{2\pi\mu_0} \frac{\partial}{\partial \psi} \left[\frac{g_2}{F} \frac{\partial \psi}{\partial V} \right] - \frac{\partial V}{\partial \psi} \langle \mathbf{j}_{ni} \cdot \mathbf{B} \rangle \tag{2}$$

We can then re-write this with ψ or Φ or ρ as independent variable:

2.1 Φ

$\hat{\Phi} = \Phi/\Phi_b$, always [0,1]

$$\sigma_\parallel \left(\left.\frac{\partial \psi}{\partial t}\right|_{\hat{\Phi}} - \frac{\hat{\Phi}\dot{\Phi}_b}{\Phi_b} \frac{\partial \psi}{\partial \hat{\Phi}} \right) = \frac{F^2}{4\pi^2\mu_0\Phi_b^2} \frac{\partial}{\partial \hat{\Phi}} \left[g_2 g_3 \frac{\partial \psi}{\partial \hat{\Phi}} \right] - \frac{1}{\Phi_b} \frac{\partial V}{\partial \hat{\Phi}} \langle \mathbf{j}_{ni} \cdot \mathbf{B} \rangle \tag{3}$$

Which is equal to E. Fable's notes [2].

2.2 ρ

$\rho = \sqrt{\Phi/\pi B_0}, d\Phi = 2\pi B_0 \rho d\rho$, and $\hat{\rho} = \sqrt{\hat{\Phi}} = \sqrt{\Phi/\Phi_b}, d\Phi = 2\Phi_b \hat{\rho} d\hat{\rho}$

$$\sigma_\| \left(\left.\frac{\partial \psi}{\partial t}\right|_\rho - \frac{\rho \dot{B}_0}{2B_0}\frac{\partial \psi}{\partial \rho} \right) = \frac{F^2}{16\pi^4 \mu_0 B_0^2 \rho}\frac{\partial}{\partial \rho}\left[\frac{g_2 g_3}{\rho}\frac{\partial \psi}{\partial \rho}\right] - \frac{1}{2\pi\rho}\frac{\partial V}{\partial \rho}\frac{\langle \mathbf{j}_{ni}\cdot \mathbf{B}\rangle}{B_0} \tag{4}$$

Which is equal to [3] since $\frac{G_2}{J} = \frac{R_0}{16\pi^4}\frac{g_2 g_3}{\rho}$

$$\sigma_\| \left(\left.\frac{\partial \psi}{\partial t}\right|_{\hat{\rho}} - \frac{\hat{\rho}\dot{\Phi}_b}{2\Phi_b}\frac{\partial \psi}{\partial \hat{\rho}} \right) = \frac{F^2}{16\pi^2 \mu_0 \Phi_b^2 \hat{\rho}}\frac{\partial}{\partial \hat{\rho}}\left[\frac{g_2 g_3}{\hat{\rho}}\frac{\partial \psi}{\partial \hat{\rho}}\right] - \frac{B_0}{2\Phi_b\hat{\rho}}\frac{\partial V}{\partial \hat{\rho}}\frac{\langle \mathbf{j}_{ni}\cdot \mathbf{B}\rangle}{B_0} \tag{5}$$

This can be rewritten to have all terms correspond to a flux-surface-averaged $\mathbf{j}\cdot\mathbf{B}$ term:

$$\underbrace{\sigma_\| \left(\frac{2\Phi_b\hat{\rho}}{V'_{\hat{\rho}}}\left.\frac{\partial \psi}{\partial t}\right|_{\hat{\rho}} - \frac{\hat{\rho}^2\dot{\Phi}_b}{V'_{\hat{\rho}}}\frac{\partial \psi}{\partial \hat{\rho}} \right)}_{\langle \mathbf{j}_\Omega \cdot \mathbf{B}\rangle} = \underbrace{\frac{F^2}{8\pi^2 \mu_0 \Phi_b V'_{\hat{\rho}}}\frac{\partial}{\partial \hat{\rho}}\left[\frac{g_2 g_3}{\hat{\rho}}\frac{\partial \psi}{\partial \hat{\rho}}\right]}_{\langle \mathbf{j}\cdot\mathbf{B}\rangle} - \langle \mathbf{j}_{ni}\cdot \mathbf{B}\rangle \tag{6}$$

2.3 Finite Element forms

$$\sigma_\| \left(\left.\frac{\partial \psi}{\partial t}\right|_{\hat{\rho}} - \frac{\hat{\rho}\dot{\Phi}_b}{2\Phi_b}\frac{\partial \psi}{\partial \hat{\rho}} \right) = \frac{F^2}{16\pi^2 \mu_0 \Phi_b^2 \hat{\rho}}\frac{\partial}{\partial \hat{\rho}}\left[\frac{g_2 g_3}{\hat{\rho}}\frac{\partial \psi}{\partial \hat{\rho}}\right] - \frac{B_0}{2\Phi_b\hat{\rho}}V'_{\hat{\rho}} j_{ni} \tag{7}$$

is rewritten to eliminate the term in front of the second order derivative, yielding

$$\frac{16\pi^2\mu_0\Phi_b^2\hat{\rho}\sigma_\|}{F^2}\left.\frac{\partial \psi}{\partial t}\right|_{\hat{\rho}} = \frac{\partial}{\partial \hat{\rho}}\left[\frac{g_2 g_3}{\hat{\rho}}\frac{\partial \psi}{\partial \hat{\rho}}\right] + \dot{\Phi}_b\frac{8\pi^2\mu_0\Phi_b\hat{\rho}^2\sigma_\|}{F^2}\frac{\partial \psi}{\partial \hat{\rho}} - \frac{8\pi^2\mu_0\Phi_b V'_{\hat{\rho}}}{F^2}\langle \mathbf{j}_{ni}\cdot \mathbf{B}\rangle \tag{8}$$

or

$$m_\psi \frac{\partial \psi}{\partial t} = a_\psi \frac{\partial \psi}{\partial \hat{\rho}} + \frac{\partial}{\partial \hat{\rho}} d_\psi \frac{\partial \psi}{\partial \hat{\rho}} + s_\psi \tag{9}$$

with

$$m_\psi = 16\pi^2\mu_0\hat{\rho}\frac{\Phi_b^2\sigma_\|}{F^2} \tag{10}$$

$$a_\psi = 8\pi^2\mu_0\dot{\Phi}_b\Phi_b\frac{\sigma_\|\hat{\rho}^2}{F^2} \tag{11}$$

$$d_\psi = \frac{g_2 g_3}{\hat{\rho}} \tag{12}$$

$$s_\psi = -8\pi^2\mu_0\Phi_b\frac{V'_{\hat{\rho}}}{F^2}\langle \mathbf{j}_{ni}\cdot \mathbf{B}\rangle \tag{13}$$

$$\tag{14}$$

Now write ψ as a sum of spatial basis functions

$$\psi(\rho, t) = \sum_{\alpha=1}^{n_{sp}} \Lambda_\alpha(\hat{\rho})\hat{y}_\alpha(t) \tag{15}$$

then the weak form, after projection on Λ_b and integration by parts is

$$\sum_{\alpha=1}^{n_{sp}} \frac{\mathrm{d}\hat{y}_\alpha(t)}{\mathrm{d}t} \int_0^1 m\Lambda_\beta \Lambda_\alpha \mathrm{d}\hat{\rho} = \sum_{\alpha=1}^{n_{sp}} \hat{y}_\alpha \int_0^1 a_\psi \Lambda_\beta \frac{\partial \Lambda_\alpha}{\partial \hat{\rho}} \mathrm{d}\hat{\rho} \tag{16}$$

$$-\sum_{\alpha=1}^{n_{sp}} \hat{y}_\alpha \int_0^1 d_\psi \frac{\partial \Lambda_\beta}{\partial \hat{\rho}} \frac{\partial \Lambda_\alpha}{\partial \hat{\rho}} \mathrm{d}\hat{\rho} + \left[d_\psi \Lambda_\beta \frac{\partial \psi}{\partial \hat{\rho}} \right]_0^1 + \int_0^1 \Lambda_\beta s_\psi \mathrm{d}\hat{\rho} \tag{17}$$

which gives the matrix form

$$\mathbf{M}_\psi \frac{\mathrm{d}\hat{\psi}}{\mathrm{d}t} = (-\mathbf{D}_\psi + \mathbf{A}_\psi)\hat{\psi} + \mathbf{l} + \mathbf{s} \tag{18}$$

The boundary term $\mathbf{l}$ contains only the last element

$$d_\psi \Lambda_\beta \frac{\partial \psi}{\partial \hat{\rho}} \bigg]_{\rho=1} = \frac{g_2 g_3}{\hat{\rho}} \frac{\partial \psi}{\partial \hat{\rho}} \bigg]_{\rho=1} = \frac{16\pi^3 \mu_0 \Phi_b}{F} \bigg]_{\rho=1} I_p \tag{19}$$

3 Thermal transport

Equation for thermal transport

$$\frac{3}{2}(V'_\rho)^{-5/3}\left(\frac{\partial}{\partial t}\bigg|_\rho - \frac{\dot{B}_0}{2B_0}\frac{\partial}{\partial \rho}\rho\right)[(V'_\rho)^{5/3} n_e T_e] + \frac{1}{V'_\rho}\frac{\partial}{\partial \rho}\left(-\frac{g_1}{V'_\rho} n_e \chi_e \frac{\partial T_e}{\partial \rho} + \frac{5}{2} T_e \Gamma_e g_0\right) = P_e \tag{20}$$

or

$$\frac{3}{2}(V'_{\hat{\rho}})^{-5/3}\left(\frac{\partial}{\partial t}\bigg|_{\hat{\rho}} - \frac{\dot{\Phi}_b}{2\Phi_b}\frac{\partial}{\partial \hat{\rho}}\hat{\rho}\right)[(V'_{\hat{\rho}})^{5/3} n_e T_e] + \frac{1}{V'_{\hat{\rho}}}\frac{\partial}{\partial \hat{\rho}}\left(-\frac{g_1}{V'_{\hat{\rho}}} n_e \chi_e \frac{\partial T_e}{\partial \hat{\rho}} + \frac{5}{2} T_e \Gamma_e g_0\right) = P_e \tag{21}$$

Where Γ_e is the electron particle flux defined in (36), in units of $\mathrm{m}^{-2}\mathrm{s}^{-1}$. The equation is rewritten as

$$\begin{aligned} \frac{3}{2} V'_{\hat{\rho}} n_e \frac{\partial T_e}{\partial t} &= \frac{\partial}{\partial \hat{\rho}}\left(\left[\frac{3}{2}\frac{\dot{\Phi}_b}{2\Phi_b} V'_{\hat{\rho}} \hat{\rho} n_e - \frac{5}{2}\Gamma_e g_0\right] T_e\right) + \frac{\partial}{\partial \hat{\rho}}\left(\frac{g_1}{V'_{\hat{\rho}}} n_e \chi_e \frac{\partial T_e}{\partial \hat{\rho}}\right) \\ &\quad + \left(\frac{\dot{\Phi}_b}{2\Phi_b}\hat{\rho} n_e \frac{\partial V'_{\hat{\rho}}}{\partial \hat{\rho}} - \frac{5}{2} n_e \frac{\partial V'_{\hat{\rho}}}{\partial t} - \frac{3}{2} V'_{\hat{\rho}} \frac{\partial n_e}{\partial t}\right) T_e + V'_{\hat{\rho}} P_e \end{aligned} \tag{22}$$

3.1 Finite Element forms

Equation in matrix form

$$m_{T_e} \frac{\partial T_e}{\partial t} = \frac{\partial}{\partial \hat{\rho}}(a_{T_e} T_e) + \frac{\partial}{\partial \hat{\rho}} d_{T_e} \frac{\partial T_e}{\partial \hat{\rho}} + h_{T_e} T_e + s_{T_e} \tag{23}$$

with

$$m_{T_e} = \frac{3}{2}V'_{\hat\rho}n_e \tag{24}$$

$$a_{T_e} = \frac{3}{2}\hat\rho n_e V'_{\hat\rho}\frac{\dot\Phi_b}{2\Phi_b} - \frac{5}{2}\Gamma_e g_0 \tag{25}$$

$$d_{T_e} = \frac{g_1}{V'_{\hat\rho}}n_e\chi_e \tag{26}$$

$$h_{T_e} = \frac{\dot\Phi_b}{2\Phi_b}\hat\rho n_e\frac{\partial V'_{\hat\rho}}{\partial\hat\rho} - \frac{5}{2}n_e\frac{\partial V'_{\hat\rho}}{\partial t} - \frac{3}{2}V'_{\hat\rho}\frac{\partial n_e}{\partial t} \tag{27}$$

$$s_{T_e} = V'_{\hat\rho}P_e \tag{28}$$

Now write T_e as a sum of spatial basis functions

$$T_e(\hat\rho,t) = \sum_{\alpha=1}^{n_{sp}}\Lambda_\alpha(\hat\rho)\hat z_\alpha(t) \tag{29}$$

then the weak form, after projection on Λ_b and integration by parts is

$$\sum_{\alpha=1}^{n_{sp}}\frac{\mathrm{d}\hat z_\alpha(t)}{\mathrm{d}t}\int_0^1 m_{T_e}\Lambda_\beta\Lambda_\alpha\mathrm{d}\hat\rho = -\sum_{\alpha=1}^{n_{sp}}\hat z_\alpha\int_0^1 a_{T_e}\frac{\partial\Lambda_\beta}{\partial\hat\rho}\Lambda_\alpha\mathrm{d}\hat\rho + [a_{T_e}\Lambda_\beta T_e]_0^1 \tag{30}$$

$$-\sum_{\alpha=1}^{n_{sp}}\hat z_\alpha\int_0^1 d_{T_e}\frac{\partial\Lambda_\beta}{\partial\hat\rho}\frac{\partial\Lambda_\alpha}{\partial\hat\rho}\mathrm{d}\hat\rho + \left[d_{T_e}\Lambda_\beta\frac{\partial T_e}{\partial\hat\rho}\right]_0^1 \tag{31}$$

$$+\sum_{\alpha=1}^{n_{sp}}\hat z_\alpha\int_0^1 h_{T_e}\Lambda_\beta\Lambda_\alpha\partial\hat\rho + \int_0^1\Lambda_\beta s_{T_e}\mathrm{d}\hat\rho \tag{32}$$

which gives the matrix form

$$\mathbf{M}_{T_e}\frac{\mathrm{d}\hat T_e}{\mathrm{d}t} = (-\mathbf{A}_{T_e} - \mathbf{D}_{T_e} + \mathbf{H}_{T_e})\hat T_e + \mathbf{l} + \mathbf{s} \tag{33}$$

with the boundary term

$$l = a_{T_e}\Lambda_\beta T_e]_{\hat\rho=1} + d_{T_e}\Lambda_\beta\frac{\partial T_e}{\partial\hat\rho}\Big]_{\hat\rho=1} = \left(\left(\frac{3}{2}\hat\rho n_e V'_{\hat\rho}\frac{\dot\Phi_b}{2\Phi_b} - \frac{5}{2}\Gamma_e g_0\right)T_e + \frac{g_1}{V'_{\hat\rho}}n_e\chi_e\frac{\partial T_e}{\partial\hat\rho}\right)\Bigg]_{\hat\rho=1} \tag{34}$$

4 Particle transport

Starting from Hinton&Hazeltine [1] equation (7.30) we find the particle transport equation (for species s), where $\frac{\partial}{\partial t}$ is intended at fixed Φ surface:

$$\left.\frac{\partial}{\partial t}\right|_\Phi(V'_\rho n_s) + \frac{\partial}{\partial\rho}\left(V'_\rho\Gamma_s\right) = V'S_s \tag{35}$$

Using the definition of ρ and allowing a time-varying B_0, and expressing Γ_s (in $\mathrm{m}^{-2}\mathrm{s}^{-1}$) as

$$\Gamma_s = -\frac{g_1}{V_\rho'^2} D_s \frac{\partial n_s}{\partial \rho} + \frac{g_0}{V_\rho'} V_s n_s, \tag{36}$$

we arrive at

$$\frac{1}{V_\rho'}\left(\frac{\partial}{\partial t}\Big|_\rho - \frac{\dot{B}_0}{2B_0}\frac{\partial}{\partial \rho}\rho\right)[(V_\rho')n_s] + \frac{1}{V_\rho'}\frac{\partial}{\partial \rho}\left(-\frac{g_1}{V_\rho'}D_s\frac{\partial n_s}{\partial \rho} + g_0 V_s n_s\right) = S_s \tag{37}$$

or

$$\frac{1}{V_{\hat\rho}'}\left(\frac{\partial}{\partial t}\Big|_{\hat\rho} - \frac{\dot{\Phi}_b}{2\Phi_b}\frac{\partial}{\partial \hat\rho}\hat\rho\right)[(V_{\hat\rho}')n_s] + \frac{1}{V_{\hat\rho}'}\frac{\partial}{\partial \hat\rho}\left(-\frac{g_1}{V_{\hat\rho}'}D_s\frac{\partial n_s}{\partial \rho} + g_0 V_s n_s\right) = S_s \tag{38}$$

Where D_s is the particle diffusion, and V_s the particle pinch (positive V_s is outward pinch).

$$V_{\hat\rho}'\frac{\partial n_s}{\partial t} = \frac{\partial}{\partial \hat\rho}\left(\left[\frac{\dot{\Phi}_b}{2\Phi_b}V_{\hat\rho}'\hat\rho - V_s g_0\right] n_s\right) + \frac{\partial}{\partial \hat\rho}\left(\frac{g_1}{V_{\hat\rho}'}D_s\frac{\partial n_s}{\partial \hat\rho}\right) - \frac{\partial V_{\hat\rho}'}{\partial t}n_s + V_{\hat\rho}'S_s \tag{39}$$

4.1 Finite Element forms

Equation in matrix form

$$m_{n_s}\frac{\partial n_s}{\partial t} = \frac{\partial}{\partial \hat\rho}(a_{n_s} n_s) + \frac{\partial}{\partial \hat\rho}d_{n_s}\frac{\partial n_s}{\partial \hat\rho} + h_{n_s}n_s + s_{n_s} \tag{40}$$

with

$$m_{n_s} = V_{\hat\rho}' \tag{41}$$

$$a_{n_s} = \frac{\dot{\Phi}_b}{2\Phi_b}V_{\hat\rho}'\hat\rho - V_s g_0 \tag{42}$$

$$d_{n_s} = \frac{g_1}{V_{\hat\rho}'}D_s \tag{43}$$

$$h_{n_s} = -\frac{\partial V_{\hat\rho}'}{\partial t} \tag{44}$$

$$s_{n_s} = V_{\hat\rho}'S_s \tag{45}$$

Now write n_s as a sum of spatial basis functions

$$n_s(\hat\rho, t) = \sum_{\alpha=1}^{n_{sp}} \Lambda_\alpha(\hat\rho)\hat{y}_\alpha(t) \tag{46}$$

then the weak form, after projection on Λ_b and integration by parts is

$$\sum_{\alpha=1}^{n_{sp}} \frac{\mathrm{d}\hat{y}_\alpha(t)}{\mathrm{d}t}\int_0^1 m_{n_s}\Lambda_\beta\Lambda_\alpha \mathrm{d}\hat\rho = -\sum_{\alpha=1}^{n_{sp}}\hat{y}_\alpha\int_0^1 a_{n_s}\frac{\partial \Lambda_\beta}{\partial \hat\rho}\Lambda_\alpha \mathrm{d}\hat\rho + [a_{n_s}\Lambda_\beta n_s]_0^1 \tag{47}$$

$$-\sum_{\alpha=1}^{n_{sp}}\hat{y}_\alpha\int_0^1 d_{n_s}\frac{\partial \Lambda_\beta}{\partial \hat\rho}\frac{\partial \Lambda_\alpha}{\partial \hat\rho}\mathrm{d}\hat\rho + \left[d_{n_s}\Lambda_\beta\frac{\partial n_s}{\partial \hat\rho}\right]_0^1 \tag{48}$$

$$+\sum_{\alpha=1}^{n_{sp}}\hat{y}_\alpha\int_0^1 h_{n_s}\Lambda_\beta\Lambda_\alpha\partial\hat\rho + \int_0^1 \Lambda_\beta s_{n_s}\mathrm{d}\hat\rho \tag{49}$$

which gives the matrix form

$$\mathbf{M}_{n_s}\frac{\mathrm{d}\hat{n}_s}{\mathrm{d}t} = (-\mathbf{A}_{n_s} - \mathbf{D}_{n_s} + \mathbf{H}_{n_s})\hat{n_s} + \mathbf{l} + \mathbf{s} \tag{50}$$

with the boundary term

$$l = a_{n_s}\Lambda_\beta n_s]_{\hat{\rho}=1} + d_{n_s}\Lambda_\beta \frac{\partial n_s}{\partial \hat{\rho}}\Bigg]_{\hat{\rho}=1} = \left(\left(\frac{\dot{\Phi}_b}{2\Phi_b}V'_{\hat{\rho}}\hat{\rho} - V_s g_0\right)n_s + \frac{g_1}{V'_{\hat{\rho}}}D_s\frac{\partial n_s}{\partial \hat{\rho}}\right)\Bigg]_{\hat{\rho}=1} \tag{51}$$

4.2 Choice of boundary conditions and constraints

1. Edge source from input.
2. Change edge source to match input line average density.
3. Internal boundary condition density from input.
4. Change internal boundary condition to match reference line average density.

In all cases: transport coefficients from model.

For full discharge simulations: allow to switch BC type as a function of time.

4.3 Choice of particle species simulations

There is freedom to choose between predicting or prescribing either evolution of either the electron density or ion density.

Particle densities and Z_{eff} are linked by the relations:

$$n_e = \sum_j n_j Z_j \tag{52}$$

and

$$Z_{eff} = \sum_j \frac{n_j Z_j^2}{n_e} \tag{53}$$

If both n_e and n_i are known (either having been prescribed or predicted by solving a transport equation), then they must either exactly satisfy quasineutrality (with Z_{eff} computed trivially from (53)), or one must introduce an additional impurity species.

If one introduces one impurity species with density n_1 and known Z_1, then one can prescribe two out of these three: n_e, n_i, n_1 and the third is calculated by (52). Z_{eff} is trivially calculated from (53).

If one also prescribes Z_{eff}, then one can prescribe two out of these four: n_e, n_i, n_1, Z_{eff} and the other two are computed from (52), (53). In practice, one would usually prescibe in any case Z_{eff} or n_i/n_1 plus either n_e or n_i. These main options are described in the next section.

4.3.1 Typical choices

We list here the typical use cases we want to implement. In the list below we indicate the main ion species by n_i and any further species as n_1, n_2. Z_1, Z_2 are charges of the non-main ion species, which may be profiles to allow heavy impurities with various charge states. When there are two main ion species (e.g. D-T mixtures), then the ion with the lowest atomic number is considered as n_i and subsequent species are numbered n_1, n_2 etc.

1. n_e predicted, n_i prescribed (or) $n_i = kn_e$, prescribe Z_{eff}, hence cheating (inconsistent with (53)), and inconsistent with (52) unless $k = 1$
2. n_e predicted or prescribed, and Z_{eff} prescribed, and Z_i, Z_1 known. $\rightarrow$ Calculate n_i and n_1 from (52), (53).
3. n_1/n_i prescribed, n_e predicted or prescribed, and Z_i, Z_1 known. $\rightarrow$ Calculate n_i, n_1 from (52), (53).
4. n_1 and n_i predicted or prescribed, and Z_i, Z_1 known. $\rightarrow$ Calculate n_e, Z_{eff} from (52), (53). (D-T with $A_i = 2.5$)
5. n_1 and n_i predicted or prescribed, and Z_i, Z_1, Z_2 and Z_{eff} known $\rightarrow$ calculate n_e, n_2 from (52), (53). (Possibility for D-T)
6. N-dimensional generalizations of the above.

Further details and general possibilities are discussed in Appendix A.1

5 Geometric coefficients and quantities related to magnetic flux

5.1 Geometric coefficients from equilibrium code quantities

Equilibrium codes (e.g. LIUQE, CHEASE) return contour integrals over flux surface quantities.

Definition of the C_i coefficients in SI units:

$$\{C_0, C_1, C_2, C_3, C_4\} = \oint \{\frac{1}{R}, 1, \frac{1}{R^2}, B_p^2, R^2 B_p^2\} \frac{\mathrm{d}l_p}{B_p} \tag{54}$$

Definitions for $\frac{\partial V}{\partial \psi}$ and B_p in terms of COCOS [?]:

$$B_p = \frac{1}{(2\pi)^{e_{Bp}}} \cdot \frac{|\nabla\psi|}{R} = \frac{\sigma_{Bp}\sigma_{Ip}}{(2\pi)^{e_{Bp}}} \cdot \frac{|\nabla\psi|}{R} \tag{55}$$

$$\frac{\partial V}{\partial \psi} = \oint \sigma_{Bp}\sigma_{Ip} \cdot \frac{2\pi R}{|\nabla\psi|} \mathrm{d}l_p = (2\pi)^{1-e_{Bp}} \sigma_{Bp}\sigma_{Ip} \oint \frac{\mathrm{d}l_p}{B_p} \tag{56}$$

C_i coefficients in terms of COCOS:

$$C_0 = \oint \frac{1}{R}\frac{\mathrm{d}l_p}{B_p} = (2\pi)^{e_{Bp}} \oint \frac{\mathrm{d}l_p}{|\nabla\psi|} \tag{57}$$

$$C_1 = \oint \frac{\mathrm{d}l_p}{B_p} = (2\pi)^{e_{Bp}} \oint \frac{R\mathrm{d}l_p}{|\nabla\psi|} \tag{58}$$

$$C_2 = \oint \frac{1}{R^2}\frac{\mathrm{d}l_p}{B_p} = (2\pi)^{e_{Bp}} \oint \frac{\mathrm{d}l_p}{R|\nabla\psi|} \tag{59}$$

$$C_3 = \oint B_p^2\frac{\mathrm{d}l_p}{B_p} = \oint B_p\mathrm{d}l_p = \frac{1}{(2\pi)^{e_{Bp}}} \oint \frac{|\nabla\psi|}{R}\,\mathrm{d}l_p \tag{60}$$

$$C_4 = \oint R^2B_p^2\frac{\mathrm{d}l_p}{B_p} = \oint R^2B_p\mathrm{d}l_p = \frac{1}{(2\pi)^{e_{Bp}}} \oint R|\nabla\psi|\,\mathrm{d}l_p \tag{61}$$

If one wants to normalize with the coefficients l_d for distance and l_B for magnetic field, one would get

$$C_0^{norm} = l_B \oint \frac{1}{R}\frac{\mathrm{d}l_p}{B_p} = l_B C_0 \tag{62}$$

$$C_1^{norm} = \frac{l_B}{l_d} \oint \frac{\mathrm{d}l_p}{B_p} = \frac{l_B}{l_d} C_1 \tag{63}$$

$$C_2^{norm} = l_d l_B \oint \frac{1}{R^2}\frac{\mathrm{d}l_p}{B_p} = l_d l_B C_2 \tag{64}$$

$$C_3^{norm} = \frac{1}{l_d l_B} \oint B_p^2\frac{\mathrm{d}l_p}{B_p} = \frac{1}{l_d l_B (2\pi)^{2e_{Bp}}} \oint \frac{(\nabla\psi)^2}{R^2}\frac{\mathrm{d}l_p}{B_p} = \frac{1}{l_d l_B} C_3 \tag{65}$$

$$C_4^{norm} = \frac{1}{l_d^3 l_B} \oint R^2B_p^2\frac{\mathrm{d}l_p}{B_p} = \frac{1}{l_d^3 l_B (2\pi)^{2e_{Bp}}} \oint (\nabla\psi)^2\frac{\mathrm{d}l_p}{B_p} = \frac{1}{l_d^3 l_B} C_4 \tag{66}$$

The system (62)-(66) provides the general definition of $C_0^{norm} - C_4^{norm}$ for any coordinate conventions and any normalization. The C_i coefficients are obtained with $l_d = l_B = 1$.

6 Flux surface averaged quantities from contour integrals

6.1 General definitions in SI and COCOS

We define $\frac{\partial V}{\partial \psi}, g_1, g_2, g_3, \frac{\partial V}{\partial \hat{\rho}}, q$ in terms of $C_0 - C_4$ defined in (42)-(46) and in terms of $C_0^{norm} - C_4^{norm}$ defined in (47)-(51).

$$\frac{\partial V}{\partial \psi} = (2\pi)^{1-e_{Bp}}\sigma_{Bp}\sigma_{Ip}C_1 = (2\pi)^{1-e_{Bp}}\sigma_{Bp}\sigma_{Ip}\frac{l_d}{l_B}C_1^{norm} \tag{67}$$

$$g_1 = \left\langle (\nabla V)^2 \right\rangle = \left(\frac{\partial V}{\partial \psi}\right)^2 \cdot \left\langle (\nabla\psi)^2 \right\rangle = (2\pi)^{2(1-e_{Bp})} \oint \frac{\mathrm{d}l_p}{B_p} \cdot \oint (\nabla\psi)^2 \frac{\mathrm{d}l_p}{B_p} \tag{68}$$

$$= (2\pi)^{2(1-e_{Bp})}C_1 \cdot (2\pi)^{2e_{Bp}}C_4 = 4\pi^2 C_1 C_4 = 4\pi^2 l_d^4 \cdot C_1^{norm}C_4^{norm} \tag{69}$$

$$g_2 = \left\langle \frac{(\nabla V)^2}{R^2} \right\rangle = \left(\frac{\partial V}{\partial \psi}\right)^2 \cdot \left\langle \frac{(\nabla \psi)^2}{R^2} \right\rangle = (2\pi)^{2(1-e_{Bp})} \oint \frac{\mathrm{d}l_p}{B_p} \cdot \oint \frac{(\nabla\psi)^2}{R^2} \frac{\mathrm{d}l_p}{B_p} \tag{70}$$

$$= (2\pi)^{2(1-e_{Bp})} C_1 \cdot (2\pi)^{2e_{Bp}} C_3 = 4\pi^2 C_1 C_3 = 4\pi^2 l_d^2 \cdot C_1^{norm} C_3^{norm} \tag{71}$$

$$g_3 = \left\langle \frac{1}{R^2} \right\rangle = \oint \frac{1}{R^2} \frac{\mathrm{d}l_p}{B_p} / \oint \frac{\mathrm{d}l_p}{B_p} = \frac{C_2}{C_1} = \frac{1}{l_d^2} \frac{C_2^{norm}}{C_1^{norm}} \tag{72}$$

$$q = \frac{\sigma_{Bp}\sigma_{\rho\theta\phi}}{(2\pi)^{1-e_{Bp}}} \frac{\partial \Phi}{\partial \psi} = \frac{\sigma_{Bp}\sigma_{\rho\theta\phi}}{(2\pi)^{1-e_{Bp}}} \frac{\partial \Phi}{\partial V} \frac{\partial V}{\partial \psi} = \sigma_{Ip}\sigma_{\rho\theta\phi} \cdot C_1 \cdot \frac{1}{2\pi} \frac{\partial}{\partial V} \int \frac{F}{R^2} \mathrm{d}V \tag{73}$$

$$= \sigma_{Ip}\sigma_{\rho\theta\phi} \cdot C_1 \cdot \frac{F}{2\pi} \left\langle \frac{1}{R^2} \right\rangle = \sigma_{Ip}\sigma_{\rho\theta\phi} \frac{1}{2\pi} F C_2 = \sigma_{Ip}\sigma_{\rho\theta\phi}\sigma_{B_0} \frac{1}{2\pi} F^{norm} C_2^{norm} \tag{74}$$

$$\frac{\partial V}{\partial \hat{\rho}} = \frac{\partial V}{\partial \psi} \frac{\partial \psi}{\partial \Phi} \frac{\partial \Phi}{\partial \hat{\rho}} = (2\pi)^{1-e_{Bp}} \sigma_{Bp}\sigma_{Ip} C_1 \cdot \frac{(2\pi)^{e_{Bp}}}{\sigma_{Ip}\sigma_{Bp} F C_2} \cdot 2\Phi_b \hat{\rho} = 4\pi \frac{C_1}{FC_2} \Phi_b \hat{\rho} \tag{75}$$

$$= 4\pi \frac{l_d}{l_B} C_1^{norm} \frac{1}{F^{norm} C_2^{norm} \sigma_{B_0}} \cdot \Phi_b^{norm} l_d^2 l_B \sigma_{B_0} \hat{\rho} = 4\pi l_d^3 \frac{C_1^{norm}}{F^{norm} C_2^{norm}} \Phi_b^{norm} \hat{\rho} \tag{76}$$

Let us rewrite the find general relations

$\frac{\partial V}{\partial \psi}$	$(2\pi)^{1-e_{Bp}} \sigma_{Bp}\sigma_{Ip} C_1$	$(2\pi)^{1-e_{Bp}} \sigma_{Bp}\sigma_{Ip} \frac{l_d}{l_B} C_1^{norm}$
g_1	$4\pi^2 C_1 C_4$	$4\pi^2 l_d^4 C_1^{norm} C_4^{norm}$
g_2	$4\pi^2 C_1 C_3$	$4\pi^2 l_d^2 C_1^{norm} C_3^{norm}$
g_3	C_2/C_1	$\frac{1}{l_d^2} C_2^{norm}/C_1^{norm}$
q	$\sigma_{Ip}\sigma_{\rho\theta\phi} \frac{1}{2\pi} F C_2$	$\sigma_{Ip}\sigma_{\rho\theta\phi}\sigma_{B_0} \frac{1}{2\pi} F^{norm} C_2^{norm}$
$\frac{\partial V}{\partial \hat{\rho}}$	$4\pi \frac{C_1}{FC_2} \Phi_b \hat{\rho}$	$4\pi l_d^3 \frac{C_1^{norm}}{F^{norm} C_2^{norm}} \Phi_b^{norm} \hat{\rho}$

6.2 Behavior at LCFS for diverted plasmas

Special care needs to be taken when evaluating these quantities at the last closed flux surface for diverted plasmas. In these cases, $|\nabla\psi|$ goes to 0 along the contour (at the x-point), and the integrals may diverge. In practice, C_0,C_1,C_2 are infinite, while C_3 and C_4, which do not have $|\nabla\psi|$ in the denominator of the integrand, remain finite. For a general flux surface averaged quantity, and for a single null, it holds that

$$< Q >= Q_{x-point} \tag{77}$$

This can be understood by the fact that the $1/|\nabla\psi|$ term effectively weighs the value at the x-point infinitely more than at other points, so only that value matters for the average. For the geometric quantities described above we have:

$$g_1(\psi_b) \to \infty \quad \text{since } C_1 = \tfrac{\partial V}{\partial \psi} \to \infty \tag{78}$$

$$g_2(\psi_b) \to \infty \quad \text{since } C_1 = \tfrac{\partial V}{\partial \psi} \to \infty \tag{79}$$

$$g_3(\psi_b) = \frac{1}{R_x^2} \tag{80}$$

$$q(\psi_b) \to \infty \quad \text{since } C_2 \to \infty \tag{81}$$

$$\frac{\partial V}{\partial \hat{\rho}} = \frac{4\pi}{F} R_x^2 \Phi_b \hat{\rho} \quad \text{since } C_1/C_2 = 1/g_3 \tag{82}$$

[later we should probably compute proper limits to write how these go to infinity]

6.3 Other quantities related to magnetic flux

q/safety factor = Rotational transform / 2π. Actual rotational trasform is $\iota = 2\pi/q$, strictly speaking $1/q$ is called $\bar{\iota}$.

$$\iota = \frac{1}{q} = \frac{\partial \psi}{\partial \Phi} = \frac{\partial \rho}{\partial \Phi} \frac{\partial \hat{\rho}}{\partial \rho} \frac{\partial \psi}{\partial \hat{\rho}} = \frac{1}{2\Phi_b \hat{\rho}} \frac{\partial \psi}{\partial \hat{\rho}} \tag{83}$$

$$I_{pl} = \int j_\phi \mathrm{d}A_\phi = \int \oint j_\phi \sigma_{B_p} \sigma_{I_p} \frac{\mathrm{d}\psi}{|\nabla \psi|} \mathrm{d}l_p = \int \left\langle \frac{j_\phi}{R} \right\rangle \frac{\sigma_{B_p} \sigma_{I_p}}{(2\pi)^{e_{Bp}}} \oint \frac{\mathrm{d}l_p}{B_p} \mathrm{d}\psi = \tag{84}$$

$$\int \frac{\sigma_{B_p}}{(2\pi)^{e_{Bp}} \mu_0} \frac{4\pi^2}{V'_\rho} \frac{\partial}{\partial \rho} \left[G_2 \frac{\partial \psi}{\partial \rho} \right] \frac{\sigma_{B_p} \sigma_{I_p}}{(2\pi)^{e_{Bp}}} \oint \frac{\mathrm{d}l_p}{B_p} \mathrm{d}\psi = \frac{\sigma_{B_p}}{(2\pi)^{e_{Bp}-1} \mu_0} G_2 \frac{\partial \psi}{\partial \rho} \tag{85}$$

One could use eq. for G_2, g_2, g_3 and $\frac{\partial V}{\partial \hat{\rho}}$ to get the following equation for I_p

$$I_{pl} = \frac{\sigma_{B_p}}{(2\pi)^{e_{Bp}+2}} \frac{1}{2\mu_0 \Phi_b} F \frac{g_2 g_3}{\hat{\rho}} \frac{\partial \psi}{\partial \hat{\rho}} = \frac{\sigma_{B_p}}{(2\pi)^{e_{Bp}+2}} \frac{1}{\mu_0} \frac{F}{q} g_2 g_3 \tag{86}$$

$$j_{tor} = 2\pi R_0 \frac{\partial I_{pl}}{\partial V} = \frac{\sigma_{B_p}}{(2\pi)^{e_{Bp}+2}} \frac{2\pi R_0}{2\mu_0 \Phi_b V'_{\hat{\rho}}} \frac{\partial}{\partial \hat{\rho}} \left[F \frac{g_2 g_3}{\hat{\rho}} \frac{\partial \psi}{\partial \hat{\rho}} \right] \tag{87}$$

$j_\parallel$ (starting from [3] eq. 34), also (6)

$$j_\parallel \equiv \frac{\langle \mathbf{j} \cdot \mathbf{B} \rangle}{B_0} = \frac{2\pi}{B_0} F^2 \frac{\partial}{\partial V} \left(\frac{I_{pl}}{F} \right) = \frac{2\pi}{B_0} \frac{\sigma_{B_p}}{(2\pi)^{e_{Bp}+2}} \frac{1}{2\mu_0 \Phi_b} \frac{F^2}{V'_{\hat{\rho}}} \frac{\partial}{\partial \hat{\rho}} \left[\frac{g_2 g_3}{\hat{\rho}} \frac{\partial \psi}{\partial \hat{\rho}} \right] \tag{88}$$

6.4 Boundary conditions at LCFS for diverted plasmas

Also here care must be taken when evaluating products $g_2 g_3 \frac{\partial \psi}{\partial \rho}$ since $\frac{\partial \psi}{\partial \rho} = 0$ but $g_2 g_3 \to \infty$. Using (86):

$$\frac{g_2 g_3}{2\Phi_b \rho} \frac{\partial \psi}{\partial \rho} = \frac{g_2 g_3}{q} = \frac{(2\pi)^{e_{Bp}+2}}{\sigma_{B_p}} \frac{\mu_0 I_{pl}}{F} \tag{89}$$

Which is well-defined and finite at the edge. This is indeed what is used as the boundary condition (19).

Also, following (77):

$$j_{\|}(\psi_b) = \frac{\langle \mathbf{j} \cdot \mathbf{B} \rangle_{\psi_b}}{B_0} = \frac{j_x B_x}{B_0} \tag{90}$$

which is generally nonzero, but can be zero in special cases zero if $\sigma_{\|} = 0$ (e.g. if zero edge temperature is imposed) and j_{ni} current vanishes simultaneously.

7 RAPTOR quantities in SI units

Lets define $\frac{\partial V}{\partial \psi}, g_1, g_2, g_3, \frac{\partial V}{\partial \hat{\rho}}, q$ for RAPTOR in terms of $C_0 - C_4$, F, Φ_b.
RAPTOR: $l_d = 1$, $l_B = 1$, $e_{Bp} = 1$, $\sigma_{B_p} = 1$, $\sigma_{I_p} = 1$, $\sigma_{R\phi Z} = 1$ $\sigma_{\rho\theta\phi} = 1$, $\sigma_{B_0} = 1$, $COCOS = 11$.

$\frac{\partial V}{\partial \psi}$	C_1
g_1	$4\pi^2 C_1 C_4$
g_2	$4\pi^2 C_1 C_3$
g_3	C_2/C_1
q	$\frac{1}{2\pi} F C_2$
$\frac{\partial V}{\partial \hat{\rho}}$	$4\pi \frac{C_1}{F C_2} \Phi_b \hat{\rho}$

The same way one could define I_{pl}, j_{tor}, $j_{\|}$ for RAPTOR.

I_{pl}	$\frac{1}{8\pi^3 \mu_0} \frac{1}{2\Phi_b} F \frac{g_2 g_3}{\hat{\rho}} \frac{\partial \psi}{\partial \hat{\rho}} = \frac{g_2 g_3}{8\pi^3 \mu_0} \frac{F}{q}$
j_{tor}	$\frac{2\pi R_0}{16\pi^3 \mu_0 \Phi_b V'_{\hat{\rho}}} \frac{\partial}{\partial \hat{\rho}} \left[F \frac{g_2 g_3}{\hat{\rho}} \frac{\partial \psi}{\partial \hat{\rho}} \right]$
$j_{\|}$	$\frac{2\pi}{B_0} \frac{1}{16\pi^3 \mu_0 \Phi_b} \frac{F^2}{V'_{\hat{\rho}}} \frac{\partial}{\partial \hat{\rho}} \left[\frac{g_2 g_3}{\hat{\rho}} \frac{\partial \psi}{\partial \hat{\rho}} \right]$

One could calculate the $C_0 - C_4$ coefficients, F, Φ_b in terms of CHEASE outputs for example.
CHEASE: $l_d = R_0$, $l_B = B_0$, $e_{Bp} = 0$, $\sigma_{B_p} = 1$, $\sigma_{I_p} = 1$, $\sigma_{\rho\theta\phi} = 1$, $\sigma_{B_0} = 1$, $COCOS = 2$.

$$C_0 = \frac{1}{B_0} C_0^{CH} \tag{91}$$

$$C_1 = \frac{R_0}{B_0} C_1^{CH} \tag{92}$$

$$C_2 = \frac{1}{R_0 B_0} C_2^{CH} \tag{93}$$

$$C_3 = R_0 B_0 C_3^{CH} \tag{94}$$

$$C_4 = R_0^3 B_0 C_4^{CH} \tag{95}$$

$$F = R_0 B_0 F^{CH} \tag{96}$$

$$\Phi_b = R_0^2 B_0 \Phi_b^{CH} \tag{97}$$

8 Plasma pressures

Many definitions exist for the plasma pressures that make use of the volume integrated thermal pressure defined by $\langle p \rangle_V = \frac{\int p dV}{\int dV} = \frac{\int p dV}{V}$. RAPTOR includes in the output function three formulations:

- Experimental: $\beta_{exp} = \frac{\langle p \rangle_V}{B_0^2/(2\mu_0)}$, (multiplied by 100 in RAPTOR to get a value close to 1)
- Normalized: $\beta_N = 100 \frac{\beta_{exp}}{I_p[\mathrm{MA}]\mathrm{B}_0[\mathrm{T}]\mathrm{a}[\mathrm{m}]}$
- Poloidal: $\beta_p = \frac{8}{3} \frac{W_{\mathrm{th}}}{\mu_0 R_0 I_p^2}$.
  A (brief) derivation:
  - Start: $\beta_p = \frac{\langle p \rangle_V}{\bar{B}_p^2/(2\mu_0)}$, with $\bar{B}_p$ an averaged poloidal magnetic field to be defined.
  - We use the definition: $\bar{B}_p = \frac{\int B_p dl_p}{\int dl_p} = \frac{\mu_0 I_p}{\int dl_p}$, where $\int dl_p$ can be either calculated by the equilibrium code or approximated.
  - Gives: $\beta_p = \frac{\langle p \rangle_V}{\frac{\mu_0 I_p^2}{2(\int dl_p)^2}}$
  - We use large aspect ratio approximation and elongated cylindrical cross section for the volume $V = 2\pi^2 R_0 a^2 \kappa$ and for the perimeter we use $(\int dl_p) = \sqrt{\frac{2V}{R_0}} = \int dl_p = 2\pi a \sqrt{\kappa}$
  - Hence we can approximate the averaged poloidal magnetic field by: $\bar{B}_p^2 = \frac{\mu_0^2 I_p^2}{\frac{2V}{R_0}}$
  - Thus inserting $\bar{B}_p^2$ in β_p: $\beta_p = \frac{\langle p \rangle_V}{\frac{\mu_0^2 I_p^2}{\frac{2V}{R_0}}/(2\mu_0)}$
  - Rewriting gives: $\beta_p = \frac{4\langle p \rangle_V V}{\mu_0 R_0 I_p^2}$
  - Using the relation: $\langle p \rangle_V = \frac{2}{3} \frac{W_{th}}{V}$
  - Finally we get: $\beta_p = \frac{8}{3} \frac{W_{\mathrm{th}}}{\mu_0 R_0 I_p^2}$

9 Neoclassical Tearing Modes

RAPTOR contains an NTM *prescribed* module for which entries in v_k hold the island width w for four modes (default: $q = \left\{\frac{2}{1}, \frac{3}{2}, \frac{4}{3}, \frac{3}{1}\right\}$). Additionally there is the NTM *mre* module which include states for the NTM width w (default: $q = \left\{\frac{2}{1}, \frac{3}{2}\right\}$). In both cases, the width w affects the thermal conductivity χ_e in the same way, following:

$$\chi_e(\rho) = \chi_{e,0}(\rho) \prod_{i=1}^{N_{NTMs}} \left(1 + A_i \exp\left[\frac{-4\left(\rho - \rho_i\right)^2}{\left(Cw_i * w_i/a\right)^2}\right]\right) \tag{98}$$

in which i indicates the mode, ρ_i is the position of the mode, A_i is the amplitude of the perturbation (*chiefact_A* in *ntm_mre.m*), Cw_i influences the width of the perturbation relative to the island width (*chiefact_w* in *ntm_mre.m*) , w_i is the island width of the i-th mode, and a is the minor radius of the plasma.

9.1 Modified Rutherford Equation

The modified rutherford equation (mre) is one of the options for including NTMs in the simulation. Details about the mre terms can be found in [4]. If this is used, a seed island width is read from v_k. This value is set in the state and is evaluated following the equation

$$\frac{dw}{dt} = \frac{\rho_s}{\tau_R}\left[\sum \rho_s\, \Delta'_{ii}\right], \tag{99}$$

where τ_R is the resistive time, Δ'_{ii} correspond to the various terms, and

$$\rho_s = \bar{\rho} = \hat{\rho}\, a \text{ [m]}. \tag{100}$$

The resistive time is taken as

$$\tau_R = \frac{\mu_0\, \rho_s^2}{1.22\, \eta_{neo}}, \tag{101}$$

where η_{neo} is the neoclassical resistivity at the rational surface and a factor (*resis_fact*) is introduced to reduce or increase local resistivity with respect to the resistivity calculated by the *sigma_neo* module in RAPTOR.

The classical growth is implemented as equation (27) in [4], with α and $\bar{\rho}_{mn}\Delta'_0$ as parameters. The default value for $\bar{\rho}_{mn}\Delta'_0$ is $-m$. In the square root a small number is added such that in case $\bar{\rho}_{mn}\Delta'_0 = -m$ and $\alpha = 0$ a division by zero does not occur.

The bootstrap current term is implemented as equation (20) in [4]. The value for f_{bse} is obtained by calling *jBSdotB*, and the values $w_{d,e}$, $w_{d,i}$, and a_2 are parameters. For $j_{bs,mn}$ an average value is used such that an unperturbed bootstrap current is taken.

The Glasser-Greene-Johnson term is implemented as equation (35), which is multiplied by a correction factor *a_ggj*. The factor *a_ggj* should normally be one, but setting it to zero will switch off the GGJ term. The value of L_{bs} is obtained from the value of L_{31} that is calculated in *jBSdotB*.

The current drive term is included following equation (39) in [4], using equations (41) and (42) for the effect of finite island width compared to current drive width and the effect of misalignment respectively. The current drive density j_{cd0} is calculated using the *echcd_gaussian* module of RAPTOR. NTM suppression requires a narrower current drive than what a typical RAPTOR simulation uses. Therefore, the peak current drive is recalculated for a width $w_{cd,NTM}$ (input parameter) under the assumption that the total driven current with the larger RAPTOR current drive width is the same.

A Further notes

A.1 Notes on choices and settings for particle transport

[JC notes, to be refined]

For a simulation with a single ion species, Z_{eff} is not prescribed, but trivially calculated. Both Z_{eff} and Z_i are profiles. Two Z_{eff} arrays are provided: one for prescribed Z_{eff} (e.g. from experimental data), and the other for calculated Z_{eff}

and is written over during the simulation, necessary for when ion species are predicted or separately prescribed (see below). Z_i is a profile to allow for heavy impurities, under the bundling assumption (at each radial location, average over all charge states). We allow up to 10 ion species to be present (Note (JC): this is to allow, for example, D+T+He3+He4+FastD+FastHe4+FastHe3+W+Kr+Be, which is the most imaginable to ever include).

For non-predicted (interpretative) ion species, we must constrain the densities by setting their ratios either with respect to n_e, or one of the other ion species. We restrict the possible ratios to one of the following:

$$C_i = n_i/n_e \tag{102}$$

$$\tilde{C}_i = n_i/n_1 \tag{103}$$

Where n_1 is the first ion species. For example, C_i is useful to constrain minority species used for ICRH heating, which is typically prescribed with respect to n_e. On the other hand, $\tilde{C}_i$ may be useful for prescribing $n_D = n_T$, for example. C_i and $\tilde{C}_i$ cannot be set together, and the simulation will not start if this inconsistency is present. If neither C_i or $\tilde{C}_i$ are set, then the Z_{eff} constraint is used for that species. This is covered more in detail below.

A.1.1 Predicted electron density

The transport model provides the transport coefficients for electron particle transport. n_e is thus known, and all ion species are interpretative. For simplicity, n_1 is always considered unknown (i.e. one cannot set C_1). There is then freedom to set one other ion species unknown and constrain it with Z_{eff}, or otherwise prescribe the ratios of all other ion species and then calculate Z_{eff} based on that.

If all ion ratios are prescribed, then the n_1 ion density is simply from quasineutrality:

$$n_1 = n_e \frac{(1 - \sum_i Z_i C_i)}{Z_1 + \sum_j \tilde{C}_j Z_j} \tag{104}$$

Where C_i and $\tilde{C}_j$ are the two types of ion density ratio. Of course, one can restrict themselves to purely using either C_i or $\tilde{C}_j$. If C_i is too large, the result may be unphysical (negative n_1). A check is set up, and simulation aborts with the appropriate warning if this occurs. Z_{eff} is calculated according to Eq. 53.

When an additional ion species apart from n_1 is not prescribed, i.e. no value for C or $\tilde{C}$ is set, then we solve its density according to both quasineutrality and the prescribed Z_eff. We name this additional unknown ion species n_u, and obtain the following matrix equation.

$$\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix} \begin{bmatrix} n_1 \\ n_u \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{105}$$

With:

$$a_1 = Z_1 + \sum_j Z_j \tilde{C}_j \tag{106}$$

$$b_1 = Z_u \tag{107}$$

$$a_2 = Z_1^2 + \sum_j Z_j^2 \tilde{C}_j \tag{108}$$

$$b_2 = Z_u^2 \tag{109}$$

$$c_1 = 1 - \sum_i Z_i \tilde{C}_i \tag{110}$$

$$c_2 = Z_{eff} - \sum_i Z_i^2 \tilde{C}_i \tag{111}$$

The standard solution is:

$$n_1 = D_x / D \tag{112}$$

$$n_u = D_y / D \tag{113}$$

With:

$$D = a_1 b_2 - b_1 a_2 \tag{114}$$

$$D_x = c_1 b_2 - b_1 c_2 \tag{115}$$

$$D_y = a_1 c_2 - c_1 a_2 \tag{116}$$

We then set $n_i = C_i n_e$ and $n_j = \tilde{C}_j n_1$, for all the other species.

A.1.2 Predicted ion density

The transport model provides the transport coefficients for ion particle transport. Some (or all) of the ions are predicted, and the rest are interpretative. For simplicity, we assume that n_1 is always predicted in this mode.

If all ion species are either predicted or prescribed with C_i and C_j ratios, then n_e is the only unknown:

$$n_e = \frac{\sum_k Z_k n_k + \sum_j Z_j n_1 \tilde{C}_j}{1 - \sum_i Z_i C_i} \tag{117}$$

Where n_k are all the known (predicted) ion species, including n_1. After calculation of n_e, we then set $n_i = C_i n_e$ and $n_j = \tilde{C}_j n_1$, for all the other ion species, as well as Z_{eff}.

When we include an unknown ion species, constrained by the prescribed Z_{eff}, we then obtain a similar matrix as before:

$$\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix} \begin{bmatrix} n_e \\ n_u \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{118}$$

Now with:

$$a_1 = -\left(1 - \sum_i Z_i \tilde{C}_i\right) \tag{119}$$

$$a_2 = -\left(Z_{eff} - \sum_i Z_i^2 \tilde{C}_i\right) \tag{120}$$

$$b_1 = Z_u \tag{121}$$

$$b_2 = Z_u^2 \tag{122}$$

$$c_1 = -\left(Z_1 + \sum_j Z_j \tilde{C}_j\right) \tag{123}$$

$$c_2 = -\left(Z_1^2 + \sum_j Z_j^2 \tilde{C}_j\right) \tag{124}$$

And again the standard solution is:

$$n_1 = D_x/D \tag{125}$$

$$n_u = D_y/D \tag{126}$$

With:

$$D = a_1 b_2 - b_1 a_2 \tag{127}$$

$$D_x = c_1 b_2 - b_1 c_2 \tag{128}$$

$$D_y = a_1 c_2 - c_1 a_2 \tag{129}$$

We then set $n_i = C_i n_e$ and $n_j = \tilde{C}_j n_1$, for all the interpretative ion species.

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