1 Software

- Dedalus v2
  Documentation `https://dedalus-project.readthedocs.io/en/v2_master/`
- Python 3.8.6

2 Equations

2.1 Most general case

Governing equations

$$\lambda_\rho \frac{\mathrm{d}}{\mathrm{d}z}\left(f^s \rho^s u^s\right) = \dot{m}^s, \tag{1a}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(f^l \rho^l u^l\right) = -\dot{m}^s, \tag{1b}$$

$$\rho^l f^l \left(\xi^l u^l - \frac{\tau}{B\,Pr}\left(\frac{\mathrm{d}\xi^l}{\mathrm{d}z} + \alpha^l_\xi \chi D \frac{1}{\rho^l}\frac{\xi^l}{T}\frac{\mathrm{d}p}{\mathrm{d}z}\right)\right) = \Sigma^l_\xi, \tag{1c}$$

$$\left(\bar{c}_p \bar{\rho}\frac{\mathrm{d}T}{\mathrm{d}z} - \alpha^* D \bar{\alpha} T \frac{\mathrm{d}p}{\mathrm{d}z}\right)\bar{u} - \frac{\dot{m}^s}{St} + \frac{\lambda_\rho}{St}\frac{j_z}{T}\frac{\mathrm{d}T}{\mathrm{d}z} = \frac{1}{B\,Pr}\frac{\mathrm{d}}{\mathrm{d}z}\left(\bar{k}\frac{\mathrm{d}T}{\mathrm{d}z}\right) + \Psi, \tag{1d}$$

$$\lambda_\rho f^s \rho^s u^s \frac{\mathrm{d}u^s}{\mathrm{d}z} + \frac{1}{2}\dot{m}^s \Delta u_z = -f^s \frac{\mathrm{d}p}{\mathrm{d}z} - \lambda_\rho f^s \rho^s - K j_z + \frac{4}{3}\frac{\lambda_\mu}{B}\frac{\mathrm{d}}{\mathrm{d}z}\left(f^s \frac{\mathrm{d}u^s}{\mathrm{d}z}\right), \tag{1e}$$

$$f^l \rho^l u^l \frac{\mathrm{d}u^l}{\mathrm{d}z} + \frac{1}{2}\dot{m}^s \Delta u_z = -f^l \frac{\mathrm{d}p}{\mathrm{d}z} - f^l \rho^l + K j_z + \frac{4}{3}\frac{1}{B}\frac{\mathrm{d}}{\mathrm{d}z}\left(f^l \frac{\mathrm{d}u^l}{\mathrm{d}z}\right), \tag{1f}$$

$$\left(\frac{1}{\lambda_\rho \rho^s} - \frac{1}{\rho^l} + \frac{\alpha^l_\xi \xi^l}{\rho^l}\right)\frac{\mathrm{d}p}{\mathrm{d}z} + \frac{1}{St\,D}\frac{1}{T}\frac{\mathrm{d}T}{\mathrm{d}z} + \frac{1}{D\chi} T \frac{\mathrm{d}\xi^l}{\mathrm{d}z} = 0, \tag{1g}$$

$$\frac{\mathrm{d}\rho^s}{\mathrm{d}z} = \rho^s \left(\lambda_\beta \beta^* \frac{\mathrm{d}p}{\mathrm{d}z} - \lambda_\alpha \alpha^* \frac{\mathrm{d}T}{\mathrm{d}z}\right), \tag{1h}$$

$$\frac{\mathrm{d}\rho^l}{\mathrm{d}z} = \rho^l \left(\beta^* \frac{\mathrm{d}p}{\mathrm{d}z} - \alpha^* \frac{\mathrm{d}T}{\mathrm{d}z} - \alpha^l_\xi \frac{\mathrm{d}\xi^l}{\mathrm{d}z}\right). \tag{1i}$$

where

$$\begin{gathered} f^l = 1 - f^s, \qquad \Delta u_z = u^s - u^l, \qquad \bar{\rho} = \lambda_\rho f^s \rho^s + f^l \rho^l, \qquad \bar{c}_p = \left(\lambda_{c_p}\lambda_\rho f^s \rho^s + f^l \rho^l\right)/\bar{\rho}, \\ \bar{\alpha} = \lambda_\alpha f^s + f^l, \qquad \bar{k} = \lambda_k f^s + f^l, \qquad \bar{u}_z = \left(\lambda_\rho f^s \rho^s u^s + f^l \rho^l u^l\right)/\bar{\rho}, \qquad \Sigma^l_\xi = \rho^l(0) f^l(0) \xi^l(0) \mathcal{U}, \\ \Psi = D\,K \frac{f^s \rho^s f^l \rho^l}{\bar{\rho}}(\Delta u_z)^2 + \frac{4D}{3B}\left\{\lambda_\mu f^s \left(\frac{\mathrm{d}u^s}{\mathrm{d}z}\right)^2 + f^l \left(\frac{\mathrm{d}u^l}{\mathrm{d}z}\right)^2\right\} + \frac{\tau\chi}{B\,Pr}\frac{f^l \rho^l \xi^l}{T}\left(\frac{1}{\chi}\frac{T}{\xi^l}\frac{\mathrm{d}\xi^l}{\mathrm{d}z} + \alpha^l_\xi D \frac{1}{\rho^l}\frac{\mathrm{d}p}{\mathrm{d}z}\right)^2. \end{gathered} \tag{2}$$

We always consider

$$\lambda_\alpha = \lambda_{c_p} = \lambda_k = 1 \tag{3}$$

thus

$$\bar{c}_p = \bar{\alpha} = \bar{k} = 1 \tag{4}$$

Boundary conditions

$$\rho^s = 1, \qquad \rho^l = 1, \qquad \frac{\mathrm{d}T}{\mathrm{d}z} = -\theta, \qquad u^s = 0, \qquad f^l u^l = -\lambda_\rho \mathcal{U} \qquad \text{on} \qquad z = 0 \tag{5}$$

$$T = 1, \qquad \xi^l = \xi_{core}, \qquad \frac{\mathrm{d}u^s}{\mathrm{d}z} = \frac{\mathrm{d}u^l}{\mathrm{d}z} = 0 \qquad \text{on} \qquad z = 1. \tag{6}$$

2.2 Simplified system

$$\mathcal{U} = 0, \qquad \Sigma^l_\xi = 0. \tag{7}$$

In this case mixture velocity is zero $\bar{u} = 0$ and thus the advection term in the heat equation vanishes.

Governing equations

$$\lambda_\rho \frac{\mathrm{d}}{\mathrm{d}z}\left(f^s\rho^s u^s\right) = \dot{m}^s, \tag{8a}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(f^l\rho^l u^l\right) = -\dot{m}^s, \tag{8b}$$

$$\xi^l u^l - \frac{\tau}{B\,Pr}\left(\frac{\mathrm{d}\xi^l}{\mathrm{d}z} + \alpha^l_\xi \chi D \frac{1}{\rho^l}\frac{\xi^l}{T}\frac{\mathrm{d}p}{\mathrm{d}z}\right) = 0, \tag{8c}$$

$$-\frac{\dot{m}^s}{St} + \frac{\lambda_\rho}{St}\frac{j_z}{T}\frac{\mathrm{d}T}{\mathrm{d}z} = \frac{1}{B\,Pr}\frac{\mathrm{d}^2T}{\mathrm{d}z^2} + \Psi, \tag{8d}$$

$$\lambda_\rho f^s\rho^s u^s\frac{\mathrm{d}u^s}{\mathrm{d}z} + \frac{1}{2}\dot{m}^s\Delta u_z = -f^s\frac{\mathrm{d}p}{\mathrm{d}z} - \lambda_\rho f^s\rho^s - Kj_z + \frac{4}{3}\frac{\lambda_\mu}{B}\frac{\mathrm{d}}{\mathrm{d}z}\left(f^s\frac{\mathrm{d}u^s}{\mathrm{d}z}\right), \tag{8e}$$

$$f^l\rho^l u^l\frac{\mathrm{d}u^l}{\mathrm{d}z} + \frac{1}{2}\dot{m}^s\Delta u_z = -f^l\frac{\mathrm{d}p}{\mathrm{d}z} - f^l\rho^l + Kj_z + \frac{4}{3}\frac{1}{B}\frac{\mathrm{d}}{\mathrm{d}z}\left(f^l\frac{\mathrm{d}u^l}{\mathrm{d}z}\right), \tag{8f}$$

$$\left(\frac{1}{\lambda_\rho\rho^s} - \frac{1}{\rho^l} + \frac{\alpha^l_\xi\xi^l}{\rho^l}\right)\frac{\mathrm{d}p}{\mathrm{d}z} + \frac{1}{St\,D}\frac{1}{T}\frac{\mathrm{d}T}{\mathrm{d}z} + \frac{1}{D\chi}T\frac{\mathrm{d}\xi^l}{\mathrm{d}z} = 0, \tag{8g}$$

$$\frac{\mathrm{d}\rho^s}{\mathrm{d}z} = \rho^s\left(\lambda_\beta\beta^*\frac{\mathrm{d}p}{\mathrm{d}z} - \lambda_\alpha\alpha^*\frac{\mathrm{d}T}{\mathrm{d}z}\right), \tag{8h}$$

$$\frac{\mathrm{d}\rho^l}{\mathrm{d}z} = \rho^l\left(\beta^*\frac{\mathrm{d}p}{\mathrm{d}z} - \alpha^*\frac{\mathrm{d}T}{\mathrm{d}z} - \alpha^l_\xi\frac{\mathrm{d}\xi^l}{\mathrm{d}z}\right). \tag{8i}$$

Boundary conditions

$$\rho^s = 1, \qquad \rho^l = 1, \qquad \frac{\mathrm{d}T}{\mathrm{d}z} = -\theta, \qquad u^s = 0, \qquad u^l = 0 \qquad \text{on} \qquad z = 0 \tag{9}$$

$$T = 1, \qquad \xi^l = \xi_{core}, \qquad \frac{\mathrm{d}u^s}{\mathrm{d}z} = \frac{\mathrm{d}u^l}{\mathrm{d}z} = 0 \qquad \text{on} \qquad z = 1. \tag{10}$$

3 Dedalus implementation

3.1 Equations - simplified

All non-linear terms have to be on the right hand side.

All equations have to be first order ODEs.

We need to include an equation

$$\frac{\mathrm{d}f^s}{\mathrm{d}z} - f^s_z = 0 \tag{11}$$

(8a), (8b) are

$$\dot{m}^s = \lambda_\rho f^s\rho^s\frac{\mathrm{d}u^s}{\mathrm{d}z} + \lambda_\rho f^s u^s\frac{\mathrm{d}\rho^s}{\mathrm{d}z} + \lambda_\rho\rho^s u^s f^s_z, \tag{12}$$

$$\dot{m}^s = -(1-f^s)\rho^l\frac{\mathrm{d}u^l}{\mathrm{d}z} - (1-f^s)u^l\frac{\mathrm{d}\rho^l}{\mathrm{d}z} + \rho^l u^l f^s_z, \tag{13}$$

Re-write (8c) as an ODE for ξ^l:

$$\frac{\mathrm{d}\xi^l}{\mathrm{d}z} - \xi^l_z = 0 \tag{14}$$

$$\xi^l_z = \frac{B\,Pr}{\tau}\xi^l u^l_z - \alpha^l_\xi\chi D\frac{1}{\rho^l}\frac{\xi^l}{T}\frac{\mathrm{d}p}{\mathrm{d}z}, \tag{15}$$

(8d) written in first order formulation

$$\frac{\mathrm{d}T}{\mathrm{d}z} - T_z = 0 \tag{16}$$

$$\begin{aligned}\frac{\mathrm{d}T_z}{\mathrm{d}z} = B\,Pr \Bigg\{ &\frac{\lambda_\rho}{St}\frac{f^s\rho^s f^l\rho^l}{\bar{\rho}T}\Delta u_z \frac{\mathrm{d}T}{\mathrm{d}z} - \frac{\dot{m}^s}{St} - D\,K\frac{f^s\rho^s f^l\rho^l}{\bar{\rho}}(\Delta u_z)^2 \\ &-\frac{4D}{3B}\left(\lambda_\mu f^s\left(\frac{\mathrm{d}u^s}{\mathrm{d}z}\right)^2 + f^l\left(\frac{\mathrm{d}u^l}{\mathrm{d}z}\right)^2\right) - \frac{\tau\chi}{B\,Pr}\frac{f^l\rho^l\xi^l}{T}\left(\frac{1}{\chi}\frac{T}{\xi^l}\frac{\mathrm{d}\xi^l}{\mathrm{d}z} + \alpha^l_\xi D\frac{1}{\rho^l}\frac{\mathrm{d}p}{\mathrm{d}z}\right)^2\Bigg\}.\end{aligned} \tag{17}$$

$$\frac{\mathrm{d}u^s}{\mathrm{d}z} - u^s_z = 0 \tag{18}$$

$$\frac{\mathrm{d}u^s_z}{\mathrm{d}z} - \frac{3\,B}{4\,\lambda_\mu}\left(\frac{\mathrm{d}P}{\mathrm{d}z} + \lambda_\rho\rho^s\right) = -\frac{1}{f^s}\frac{\mathrm{d}f^s}{\mathrm{d}z}\frac{\mathrm{d}u^s}{\mathrm{d}z} + \frac{3B}{4\,\lambda_\mu}\left(\lambda_\rho\rho^s u^s\frac{\mathrm{d}u^s}{\mathrm{d}z} + \mathcal{K}f^l\frac{\rho^s\rho^l}{\bar{\rho}}\Delta u_z + \frac{1}{2}\frac{\dot{m}^s}{f^s}\Delta u_z\right), \tag{19}$$

here, I found that the performance is better when (12) is used to substitute $\dot{m}^s$ out of the right-hand side of the equation.

Similarly,

$$\frac{\mathrm{d}u^l}{\mathrm{d}z} - u^l_z = 0 \tag{20}$$

$$\frac{\mathrm{d}u^l_z}{\mathrm{d}z} - \frac{3B}{4}\left(\frac{\mathrm{d}P}{\mathrm{d}z} + \rho^l\right) = -\frac{1}{f^l}\frac{\mathrm{d}f^l}{\mathrm{d}z}\frac{\mathrm{d}u^l}{\mathrm{d}z} + \frac{3B}{4}\left(\rho^l u^l\frac{\mathrm{d}u^l}{\mathrm{d}z} - K f^s\frac{\rho^s\rho^l}{\bar{\rho}}\Delta u_z + \frac{1}{2}\frac{\dot{m}^s}{f^l}\Delta u_z\right), \tag{21}$$

where again here, I found that the performance is better when (13) is used to substitute $\dot{m}^s$ out of the right-hand side of the equation.

The liquidus is

$$\left(\frac{1}{\rho^l} - \frac{1}{\lambda_\rho\rho^s}\right)\frac{\mathrm{d}P}{\mathrm{d}z} = \frac{\alpha^l_\xi\xi^l}{\rho^l}\frac{\mathrm{d}p}{\mathrm{d}z} + \frac{1}{St\,D}\frac{1}{T}\frac{\mathrm{d}T}{\mathrm{d}z} + \frac{1}{D\chi}T\frac{\mathrm{d}\xi^l}{\mathrm{d}z} \tag{22}$$

where the dimensionless densities are taken as constant $\rho^s = \rho^l = 1$.

Finally, equations of state which are already in the correct form

$$\frac{\mathrm{d}\rho^s}{\mathrm{d}z} = \rho^s\left(\lambda_\beta\beta^*\frac{\mathrm{d}P}{\mathrm{d}z} - \lambda_\alpha\alpha^*\frac{\mathrm{d}T}{\mathrm{d}z}\right) \tag{23}$$

$$\frac{\mathrm{d}\rho^l}{\mathrm{d}z} = \rho^l\left(\beta^*\frac{\mathrm{d}P}{\mathrm{d}z} - \alpha^*\frac{\mathrm{d}T}{\mathrm{d}z} - \alpha^l_\xi\frac{\mathrm{d}\xi^l}{\mathrm{d}z}\right) \tag{24}$$

3.2 Equations - full ($\mathcal{U} \neq 0$)

In this case it can be show that

$$\bar{\rho}\bar{u} = -\lambda_\rho\mathcal{U} \tag{25}$$

Most of the equations remain unchanged. Concentration equation (15) is modified to

$$\xi^l_z = \frac{B\,Pr}{\tau}\left(\xi^l u^l_z - \frac{\Sigma^l_\xi}{\rho^l f^l}\right) - \alpha^l_\xi\chi D\frac{1}{\rho^l}\frac{\xi^l}{T}\frac{\mathrm{d}p}{\mathrm{d}z} \tag{26}$$

Temperature equation (17) is modified to

$$\begin{aligned}\frac{\mathrm{d}T_z}{\mathrm{d}z} = B\,Pr\Bigg\{&-\lambda_\rho\mathcal{U}\left(T_z - \frac{\alpha^* DT}{\bar{\rho}}\frac{\mathrm{d}p}{\mathrm{d}z}\right) + \frac{\lambda_\rho}{St}\frac{f^s\rho^s f^l\rho^l}{\bar{\rho}T}\Delta u_z\frac{\mathrm{d}T}{\mathrm{d}z} - \frac{\dot{m}^s}{St} - D\,K\frac{f^s\rho^s f^l\rho^l}{\bar{\rho}}(\Delta u_z)^2 \\ &-\frac{4D}{3B}\left(\lambda_\mu f^s\left(\frac{\mathrm{d}u^s}{\mathrm{d}z}\right)^2 + f^l\left(\frac{\mathrm{d}u^l}{\mathrm{d}z}\right)^2\right) - \frac{\tau\chi}{B\,Pr}\frac{f^l\rho^l\xi^l}{T}\left(\frac{1}{\chi}\frac{T}{\xi^l}\frac{\mathrm{d}\xi^l}{\mathrm{d}z} + \alpha^l_\xi D\frac{1}{\rho^l}\frac{\mathrm{d}p}{\mathrm{d}z}\right)^2\Bigg\}/\end{aligned} \tag{27}$$

Σ^l_ξ is a constant that is not know a priori and needs to be determined; since it is a constant it satisfies the ODE:

$$\frac{\mathrm{d}\Sigma^l_\xi}{\mathrm{d}z} = 0. \tag{28}$$

We construct a residual variable

$$R_\xi = \Sigma_\xi^l - \rho^l f^l \xi^l \mathcal{U} \tag{29}$$

which has to satisfy the boundary condition

$$R_\xi = 0 \qquad \text{on} \qquad z = 0 \tag{30}$$

Similarly, the boundary condition on u^l is no longer no-slip and we introduce a residual variable

$$R_{u^l} = f^l u^l + \lambda_\rho \mathcal{U} \tag{31}$$

and a new boundary condition replacing the old one

$$R_{u^l} = 0 \qquad \text{on} \qquad z = 0 \tag{32}$$

3.3 Variables

- $f^s \to$ `fS`
- $f_z^s \to$ `fS_z`
- $\frac{\mathrm{d}p}{\mathrm{d}z} \to$ `Pz`
- $\dot{m}^s \to$ `mDotS`
- $u^s \to$ `uS`
- $u_z^s \to$ `uS_z`
- $u^l \to$ `uL`
- $u_z^l \to$ `uL_z`
- $T \to$ `T`
- $T_z \to$ `Tz`
- $\xi^l \to$ `Xi`
- $\xi_z^l \to$ `Xi_z`
- $\rho^s \to$ `rhoS`
- $\rho^l \to$ `rhoL`

3.4 Input parameters

- `nz` — number of grid points
- `theta` — (minus) temperature gradient on ICB (i.e. $\mathrm{d}T/\mathrm{d}z = -\theta$ on $z = 0$)
- `Pr` — Pr Prandtl number
- `St` — St Stefan number
- `D` — D Dissipation number
- `K` — K Interphase friction parameter
- `alpha` — α^* dimensionless thermal expansion parameter
- `beta` — β^* dimensionless compression parameter
- `lambda_alpha` — λ_α ratio of thermal expansion coefficients between solid and liquid phases
- `lambda_beta` — λ_β ratio of isothermal compression coefficients between solid and liquid phases
- `lambda_rho` — λ_ρ ratio of densities between solid and liquid phases
- `lambda_cp` — λ_{c_p} ratio of specific heat capacities between solid and liquid phases

- `lambda_k` — λ_k ratio of thermal conductivities between solid and liquid phases
- `chi` — χ parameter
- `alpha_xi` — α_ξ chemical expansion coefficient
- `tau` — τ ratio of chemical to thermal diffusivity
- `xi_core` — ξ_{core} core oxygen concentration
- `M` — λ_μ/B
- `B` — B buoyancy parameter
- `U_ICB` — $\mathcal{U}$ dimensionless ICB speed

3.5 Overview

Codes functions are split across 5 main modules

- `def_equations_binary.py` — defines the BVP
  - `def_equations_binary_LMOB.py` — same but with M as variable parameter
- `def_utilities.py` — various helpful functions
- `def_plotting.py` — plotting functions
- `def_diagnostics.py` — functions that loop over solution files and collect diagnostic information
- `def_analysis.py` — contains functions that calculate diagnostic quantities for a given solution and package them in a dictionary.

3.6 Procedure

- the solver function is `binaryslurryODEs` in file `def_equations_binary.py`
- `binaryslurryODEs(parameters, init_guess)` has two input arguments
  - `parameters` is a dictionary of input parameters
  - `init_guess` is a dictionary containing initial guesses for the variables
- The function returns to outputs: `solver`, and `pert_norm`
  - `solver` is a dedalus object which contain solution data
  - `pert_norm` is the residual
- Solution data needs to be extracted out of the dedalus object `solver`.
- This is done using the function `extractVars` which takes the dedalus solution object and the input parameters dictionary and returns a dictionary of all solution variables, the grid, and the parameters at which the solution was calculated. Optionally, the function also saves the output dictionary into a file.

4 Post-processing

4.1 Diagnostic quantities

- `fS_top` — solid fraction at the top $f^s(z=1)$
- `fL_top` — liquid fraction at the top $f^l(z=1) = 1 - f^s(z=1)$
- `fS_avg` — average solid fraction $\int f^s \, \mathrm{d}z$
- `fS_max` — maximum solid fraction $\max(f^s)$
- `z_fS_max` — z coordinate at which solid fraction is maximum
- `fS_min` — minimum solid fraction $\min(f^s)$
- `z_fS_min` — z coordinate at solid fraction is minimum
- `rho_top` — mixture density at the top $\bar{\rho}(z=1)$
- `rho_bot` — mixture density at the bottom $\bar{\rho}(z=1)$
- `R_rho` — ratio of density at the top versus density at the bottom $R_\rho = \bar{\rho}(z=1)/\bar{\rho}(z=0)$
- `gradRho_max` — maximum value of the density gradient $\max(\frac{\mathrm{d}\bar{\rho}}{\mathrm{d}z})$
- `z_gradRho_max` — z coordinate at which density gradient is maximised
- `uS_top` — solid velocity at the top $u^s(z=1)$
- `uS_avg` — average solid velocity $\int u^s \, \mathrm{d}z$
- `uS_scaled` — $K \langle u^s \rangle / (\lambda_\rho - 1)$
- `uS_max` — maximum absolute solid velocity $\max(|u^s|)$
- `z_uS_max` — z coordinate of the maximum absolute value of solid velocity
- `ReS_max` — Reynolds number based on the maximum solid velocity: (B/λ_μ)`uS_max`
- `ReS_avg` — Reynolds number based on the average solid velocity: $(B/\lambda_\mu)\langle u^s \rangle$
- `uL_top` — liquid velocity at the top $u^l(z=1)$
- `uL_avg` — average liquid velocity $\langle u^l \rangle = \int_0^1 u^l \, \mathrm{d}z$
- `uL_scaled` — $K \langle u^l \rangle / (\lambda_\rho - 1)$
- `uL_max` — maximum liquid velocity $\max(u^l)$
- `z_uL_max` — z coordinate at which liquid velocity is maximum
- `ReL_max` — Reynolds number based on the maximum liquid velocity: $B \max(u^l)$
- `ReL_avg` — Reynolds number based on the maximum liquid velocity: $B \langle u^l \rangle$
- `jz_avg` — average phase separation flux $\langle j_z \rangle = \int_0^1 j_z \, \mathrm{d}z$, where $j_z = \dfrac{f^s \rho^s f^l \rho^l}{\bar{\rho}} \left(u_z^s - u^l\right)$
- `jz_scaled` — $K \langle j_z \rangle$
- `mDotS_avg` —average phase change $\langle \dot{m}^s \rangle = \int_0^1 \dot{m}^s \, \mathrm{d}z$
- `rSfSuS_avg` — average solid mass flux $\int_0^1 \rho^s f^s u^s \, \mathrm{d}z$
- `rLfLuL_avg` — average liquid mass flux $\int_0^1 \rho^l f^l u^l \, \mathrm{d}z$

Momentum balance Integrating (8e)

$$\underbrace{\int_0^1 \left(\lambda_\rho f^s \rho^s u^s \frac{\mathrm{d}u^s}{\mathrm{d}z}\right) \mathrm{d}z}_{\texttt{inertiaS}} + \underbrace{\int_0^1 \frac{1}{2}\dot{m}^s \Delta u_z \,\mathrm{d}z}_{\texttt{phaseCh}} = \underbrace{\int_0^1 \left(-f^s \frac{\mathrm{d}p}{\mathrm{d}z}\right) \mathrm{d}z}_{\texttt{PzS}} + \underbrace{\int_0^1 \left(-\lambda_\rho f^s \rho^s\right) \mathrm{d}z}_{\texttt{buoyS}} - \underbrace{\int_0^1 K j_z \,\mathrm{d}z}_{\texttt{frictionL}} + \underbrace{\int_0^1 \frac{4}{3}\frac{\lambda_\mu}{B}\frac{\mathrm{d}}{\mathrm{d}z}\left(f^s \frac{\mathrm{d}u^s}{\mathrm{d}z}\right) \mathrm{d}z}_{\texttt{viscS}}, \tag{33}$$

$$\underbrace{\int_0^1 f^l \rho^l u^l \frac{\mathrm{d}u^l}{\mathrm{d}z} \,\mathrm{d}z}_{\texttt{inertiaL}} + \underbrace{\int_0^1 \frac{1}{2}\dot{m}^s \Delta u_z \,\mathrm{d}z}_{\texttt{phaseCh}} = \underbrace{\int_0^1 \left(-f^l \frac{\mathrm{d}p}{\mathrm{d}z}\right) \mathrm{d}z}_{\texttt{PzL}} + \underbrace{\int_0^1 \left(-f^l \rho^l\right) \mathrm{d}z}_{\texttt{buoyL}} + \underbrace{\int_0^1 K j_z \,\mathrm{d}z}_{\texttt{frictionL}} + \underbrace{\int_0^1 \frac{4}{3}\frac{1}{B}\frac{\mathrm{d}}{\mathrm{d}z}\left(f^l \frac{\mathrm{d}u^l}{\mathrm{d}z}\right) \mathrm{d}z}_{\texttt{viscL}}, \tag{34}$$

These diagnostic quantities are contained under keywords

- `inertiaL`
- `PzL`
- `buoyL`
- `frictionL`
- `phaseCh`
- `viscL`
- `inertiaS`
- `PzS`
- `buoyS`
- `viscS`

Heat balance The total heat balance in the 1D system, which follows from integrating the temperature equation (8d), may be written as

$$Q^C = Q^L + Q^P + Q^F + Q^{V,s} + Q^{V,l} + Q^\xi. \tag{35}$$

The term on the left hand side represents the net conductive heat flux across the slurry layer, i.e. difference between heat flux out at the top $q^C_{z=1}$ and heat flux in at the bottom $q^C_{z=0}$:

$$Q^C = \int_0^1 -\frac{\mathrm{d}}{\mathrm{d}z}\left(\bar{k}\frac{\mathrm{d}T}{\mathrm{d}z}\right)\mathrm{d}z = -\left.\left(\bar{k}\frac{\mathrm{d}T}{\mathrm{d}z}\right)\right|_{z=1} + \bar{k}\theta = q^C_{z=1} - q^C_{z=0}. \tag{36}$$

Terms on the right hand side represent contributions due to latent heat release/absorption Q^L, the heat-pipe effect Q^P, inter-phase friction Q^F, viscous heating Q^V, and heat of reaction Q^ξ:

$$\begin{aligned}
Q^L &= \frac{\sqrt{R\,Pr}}{St}\int_0^1 \dot{m}^s \,\mathrm{d}z, & Q^{V,s} &= \frac{4}{3}DPr\int_0^1 \lambda_\mu f^s \left(\frac{\mathrm{d}u^s}{\mathrm{d}z}\right)^2 \mathrm{d}z,\\
Q^P &= -\frac{\lambda_\rho\sqrt{R\,Pr}}{St}\int_0^1 \frac{j_z}{T}\frac{\mathrm{d}T}{\mathrm{d}z}\,\mathrm{d}z, & Q^{V,l} &= \frac{4}{3}DPr\int_0^1 f^l \left(\frac{\mathrm{d}u^l}{\mathrm{d}z}\right)^2 \mathrm{d}z,\\
Q^F &= D\,\mathcal{K}\sqrt{R\,Pr}\int_0^1 j_z \Delta u_z \,\mathrm{d}z, & Q^\xi &= \frac{\tau\chi}{B\,Pr}\int_0^1 \frac{f^l\rho^l\xi^l}{T}\left(\frac{1}{\chi}\frac{T}{\xi^l}\frac{\mathrm{d}\xi^l}{\mathrm{d}z} + \alpha^l_\xi D\frac{1}{\rho^l}\frac{\mathrm{d}p}{\mathrm{d}z}\right)^2 \mathrm{d}z.
\end{aligned} \tag{37}$$

- `Qc_left` - $q^C_{z=0}$
- `Qc_right` - $q^C_{z=1}$

- `Qc_ratio` - $q^C_{z=1}/q^C_{z=0}$
- `Ql` - Q^L
- `Qp` - Q^P
- `QvS` - $Q^{V,s}$
- `QvL` - $Q^{L,s}$
- `Qf` - Q^F
- `Qxi` - Q^ξ

Concentration diagnostics

- `H_xi_avg` — chemical concentration scale height $H_\xi = \left|\dfrac{1}{\xi}\dfrac{\mathrm{d}\xi}{\mathrm{d}z}\right|$
- `Xi_bot` — chemical concentration at the bottom boundary $\xi(z=0)$
- `Xi_avg` — average chemical concentration $\int_0^1 \xi \,\mathrm{d}z$
- `Xi_z_avg` — average gradient of chemical concentration $\int_0^1 (\mathrm{d}\xi/\mathrm{d}z)\,\mathrm{d}z$
- `Xi_z_bot` — gradient of chemical concentration on the bottom boundary $\mathrm{d}\xi/\mathrm{d}z(z=0)$
- `Xi_z_top` — gradient of chemical concentration on the top boundary $\mathrm{d}\xi/\mathrm{d}z(z=1)$
- `J_Xi_avg` — (modulus of) average chemical concentration flux $\left|\int_0^1 J_\xi \,\mathrm{d}z\right|$, where $J_\xi = -\frac{\tau}{B\,Pr}\rho^l f^l \left(\frac{\mathrm{d}\xi^l}{\mathrm{d}z} + \alpha^l_\xi \chi D \frac{1}{\rho^l}\frac{\xi^l}{T}\frac{\mathrm{d}p}{\mathrm{d}z}\right)$
- `J_Xi_scaled` — $\frac{B\,Pr}{\tau}\left|\int_0^1 J_\xi \,\mathrm{d}z\right|$