

Rate of change of Lithium moles

$$\frac{d}{dt} \int_{\mathcal{R}} c \rho \, dV = \frac{d}{dt} \int_{\mathcal{R}_0} \underbrace{c \rho}_{\rho_0} \det F_0 \, dV \quad F_0 \equiv \nabla \phi$$

$$= \int_{\mathcal{R}_0} (\dot{c} \rho + c \dot{\rho} + c \rho \operatorname{div} \mathbf{v}) \det F_0 \, dV$$

$$= \int_{\mathcal{R}_0} \dot{c} \rho \det F_0 \, dV + \int_{\mathcal{R}_0} \underbrace{c (\dot{\rho} + \rho \operatorname{div} \mathbf{v})}_0 \det F_0 \, dV$$

$$= \int_{\mathcal{R}_0} \dot{c} \rho_0 \, dV = \int_{\mathcal{R}} \dot{c} \rho \, dV$$

$$c = \frac{l_{\text{Li}}}{\rho_0} = \frac{\text{molar density of lithium per unit reference volume}}{\text{molar density of lattice sites per unit reference volume}}$$

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Lithium flux

$$\int_{\partial \mathcal{R}} h \cdot n \, dA = \int_{\partial \mathcal{R}_0} (h \cdot n) \frac{A_F}{A_{F_0}} \, dA = \int_{\partial \mathcal{R}_0} h \cdot (\text{cof } F_0) n_0 \, dA$$

$$= \int_{\partial \mathcal{R}_0} h \cdot F_0^{-T} n_0 (\det F_0) \, dA$$

$$= \int_{\partial \mathcal{R}_0} (\det F_0) F_0^{-1} h \cdot n_0 \, dA$$

$\underbrace{\hspace{10em}}_{h_0}$

$$= \int_{\partial \mathcal{R}_0} h_0 \cdot n_0 \, dA$$

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Species molar balance

$$\frac{d}{dt} \int_{\mathcal{R}} c_p dV = - \int_{\partial \mathcal{R}} h \cdot n d\Delta + \int_{\mathcal{R}} h dV$$

flux source

We assume $h = 0$ (no production/reaction)

$$\int_{\mathcal{R}} \dot{c}_p dV = - \int_{\partial \mathcal{R}} h \cdot n d\Delta$$

$$\int_{\mathcal{R}_0} \dot{c}_{p_0} dV = - \int_{\partial \mathcal{R}_0} h_0 \cdot n_0 d\Delta$$

which localize to

$$\dot{c}_p + \operatorname{div} h = 0 \quad \text{in } \mathcal{R}$$

$$\dot{c}_{p_0} + \operatorname{div} h_0 = 0 \quad \text{in } \mathcal{R}_0$$

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From molar balance to power balance

Let us introduce a scalar field (chemical potential)

$$\mu_0(x) = \mu(\phi(x))$$

"energy per mole of lithium"

in order to turn the species molar balance into a power molar balance:

$$\int_{\mathcal{R}} (\dot{c}\rho + \operatorname{div} h) \mu \, dV = 0 \quad \forall \mu$$

$$\int_{\mathcal{R}_0} (\dot{c}\rho_0 + \operatorname{div} h_0) \mu_0 \, dV = 0 \quad \forall \mu_0$$

$$\Rightarrow \int_{\mathcal{R}_0} \mu_0 \dot{c}\rho_0 \, dV = - \int_{\mathcal{R}_0} \operatorname{div} (\mu_0 h_0) \, dV + \int_{\mathcal{R}_0} h_0 \cdot \nabla \mu_0 \, dV = 0$$

$$\int_{\mathcal{R}_0} \mu_0 \dot{c}\rho_0 \, dV = - \int_{\partial \mathcal{R}_0} \mu_0 h_0 \cdot n_0 \, dA + \int_{\mathcal{R}_0} h_0 \cdot \nabla \mu_0 \, dV = 0$$

with

$$\begin{aligned} \operatorname{div} (\mu_0 h_0) &= \operatorname{tr} (\nabla (\mu_0 h_0)) = \operatorname{tr} (\mu_0 \nabla h_0 + \nabla \mu_0 \otimes h_0) \\ &= \mu_0 \operatorname{div} h_0 + h_0 \cdot \nabla \mu_0 \end{aligned}$$

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