

1 Mathematical Formulation

The geometry considered is a thin film of Silicon in the domain $-L/2 \leq X \leq L/2$ and $0 \leq Y \leq H$. Consider a certain particle, initially located at the coordinate \mathbf{X} . During deformation, this particle follows a path

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t) \quad (1)$$

Let $\mathbf{u}(\mathbf{X}, t)$ be the displacement of a material particle located at \mathbf{X} . Then

$$\mathbf{u}(\mathbf{X}, t) = \mathbf{x}(\mathbf{X}, t) - \mathbf{X} = [u(\mathbf{X}, t), v(\mathbf{X}, t), w(\mathbf{X}, t)]^\top \quad (2)$$

Let the deformation gradient be denoted by \mathbf{F} .

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \nabla_{\mathbf{X}} \mathbf{u} + \mathbf{I} \quad (3)$$

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^\top \mathbf{F} - \mathbf{I}) \quad (4)$$

Assuming plane strain deformation,

$$\mathbf{F} = \begin{bmatrix} 1 + \frac{\partial u}{\partial X} & \frac{\partial u}{\partial Y} & 0 \\ \frac{\partial v}{\partial X} & 1 + \frac{\partial v}{\partial Y} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} F_{11} & F_{12} & 0 \\ F_{21} & F_{22} & 0 \\ 0 & 0 & F_{33} \end{bmatrix} \quad (5)$$

Decomposition of deformation gradient

$$\mathbf{F} = \mathbf{F}^{\text{el}} \mathbf{F}^{\text{inel}} \quad (6)$$

where \mathbf{F}^{el} and \mathbf{F}^{inel} are the deformation gradients due to elastic deformation and inelastic deformation respectively.

The inelastic deformation gradient tensor, \mathbf{F}^{inel} , has contribution from two sources - Deformation due to concentration gradient and Viscoplastic deformation.

$$\mathbf{F}^{\text{inel}} = \mathbf{F}^{\text{c}} \mathbf{F}^{\text{p}} \quad (7)$$

1.1 Viscoplastic Deformation

$$\dot{\mathbf{F}}^{\text{p}} = (J)^{-1} \frac{3}{2} \frac{\mathbf{M}_0^{\text{el}} \mathbf{F}^{\text{p}}}{\sigma_{\text{eff}}} \dot{d}_0 \left(\frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right)^m \quad (8)$$

$$\mathbf{M}_0^{\text{el}} = J(\mathbf{F}^{\text{el}})^\top \boldsymbol{\tau}(\mathbf{F}^{\text{el}})^{-\top} \quad (9)$$

\mathbf{F}^{p} is assumed to be of the following form:

$$\mathbf{F}^{\text{p}} = \begin{bmatrix} \lambda_{xx} & \lambda_{xy} & 0 \\ \lambda_{yx} & \lambda_{yy} & 0 \\ 0 & 0 & \lambda_{zz} \end{bmatrix} \quad (10)$$

since, $\det(\mathbf{F}^{\text{p}}) = 1$

$$\lambda_{zz} = 1/(\lambda_{xx}\lambda_{yy} - \lambda_{xy}\lambda_{yx}) \quad (11)$$

1.2 Deformation due to concentration gradient

$$\mathbf{F}^c = (J^c)^{1/3} \mathbf{I} \quad (12)$$

$$\text{where } J^c = 1 + 3\eta\chi_{\max}\tilde{c} \quad (13)$$

$$\mathbf{F}^{\text{inel}} = \mathbf{F}^p \mathbf{F}^c \quad (14)$$

$$\mathbf{F}^{\text{el}} = \mathbf{F}(\mathbf{F}^p \mathbf{F}^c)^{-1} \quad (15)$$

$$\mathbf{E}^{\text{el}} = \frac{1}{2} [(\mathbf{F}^{\text{el}})^\top \mathbf{F}^{\text{el}} - \mathbf{I}] \quad (16)$$

Let \mathbf{P} and \mathbf{S} denote the first and second Piola-Kirchhoff stress tensors respectively.

$$W(\mathbf{F}, c) = \frac{J^c}{2} \frac{E(c)}{1 + \nu} \left(\frac{\nu}{1 - 2\nu} (\text{tr} \mathbf{E}^{\text{el}})^2 + \text{tr}(\mathbf{E}^{\text{el}} \mathbf{E}^{\text{el}}) \right) \quad (17)$$

$$\mathbf{S}^{\text{el}} = J^c [2\mu_{\text{si}}(c) \mathbf{E}^{\text{el}} + \lambda_{\text{si}}(c) \text{tr}(\mathbf{E}^{\text{el}}) \mathbf{I}] \quad (18)$$

$$\mathbf{S} = (\mathbf{F}^c)^{-1} (\mathbf{F}^p)^{-1} \mathbf{S}^{\text{el}} (\mathbf{F}^p)^{-\top} (\mathbf{F}^c)^{-\top} \quad (19)$$

$$\mathbf{P} = \mathbf{F} \mathbf{S} \quad (20)$$

Let $\boldsymbol{\sigma}$ denote the Cauchy stress tensor. Then

$$\boldsymbol{\sigma} = (J)^{-1} \mathbf{P} \mathbf{F}^\top \quad (21)$$

$$\text{where, } J = \det(\mathbf{F}) \quad (22)$$

Let $\boldsymbol{\tau}$ denote the deviatoric part of the Cauchy stress, $\boldsymbol{\sigma}$; then

$$\boldsymbol{\tau} = \boldsymbol{\sigma} - (1/3) \text{tr}(\boldsymbol{\sigma}) \mathbf{I} \quad (23)$$

$$(24)$$

Let σ_{eff} denote the von Mises stress. Then:

$$\sigma_{\text{eff}} = \sqrt{\frac{3}{2} (\tau_{11}^2 + \tau_{22}^2 + \tau_{33}^2 + 2\tau_{12}^2)} \quad (25)$$

Stress equilibrium equation:

$$\nabla_{\mathbf{X}} \cdot \mathbf{P} = 0. \quad (26)$$

Mass conservation equation:

$$\frac{\partial c}{\partial t} = -\nabla_{\mathbf{X}} \cdot \mathbf{j} \quad (27)$$

1.3 Non-Dimensionalization

$$\begin{aligned}
\tilde{c} &= c/c_{\max} & \tilde{j} &= jH/(c_{\max}D_0) \\
\text{where, } c_{\max} &= \chi_{\max}/V_m^B \\
\tilde{u} &= u/H & \tilde{v} &= v/H \\
\tilde{X} &= X/H & \tilde{Y} &= Y/H \\
\tilde{t} &= D_0t/H^2 & \tilde{\mu}_{\text{si}}, \tilde{\lambda}_{\text{si}} &= \mu_{\text{si}}/E_0, \lambda_{\text{si}}/E_0 \\
\tilde{E}(c) &= E_{\text{si}}(1 + \eta_E \chi_{\max} \tilde{c})/E_0, \text{ where } E_0 = \frac{R_g T}{V_m^b}
\end{aligned}$$

1.4 Definition of the state of charge

$$\text{soc} = \frac{\int_{-L/2}^{L/2} \int_0^H \tilde{c} dy dx}{LH} \quad (28)$$

$$= H^2 \frac{\int_{-L/2H}^{L/2H} \int_0^1 \tilde{c}(\tilde{x}, \tilde{y}) d\tilde{y} d\tilde{x}}{LH} \quad (29)$$

$$= H \frac{\int_{-L/2H}^{L/2H} \int_0^1 \tilde{c}(\tilde{x}, \tilde{y}) d\tilde{y} d\tilde{x}}{L} \quad (30)$$

$$= 2H \frac{\int_0^{L/2H} \int_0^1 \tilde{c}(\tilde{x}, \tilde{y}) d\tilde{y} d\tilde{x}}{L} \quad (31)$$

$$= \frac{2H}{L} \text{intop1}(\tilde{c}) \quad (32)$$

1.5 Equations in component form

$$\mathbf{F} = \begin{bmatrix} 1 + \frac{\partial \tilde{u}}{\partial \tilde{X}} & \frac{\partial \tilde{u}}{\partial \tilde{Y}} & 0 \\ \frac{\partial \tilde{v}}{\partial \tilde{X}} & 1 + \frac{\partial \tilde{v}}{\partial \tilde{Y}} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \tilde{F}_{11} & \tilde{F}_{12} & 0 \\ \tilde{F}_{21} & \tilde{F}_{22} & 0 \\ 0 & 0 & \tilde{F}_{33} \end{bmatrix} \quad (33)$$

$$F_{11}^{el} = \frac{F_{11} \lambda_{22} - F_{12} \lambda_{21}}{J^{c^{1/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (34)$$

$$F_{21}^{el} = \frac{F_{21} \lambda_{22} - F_{22} \lambda_{21}}{J^{c^{1/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (35)$$

$$F_{12}^{el} = -\frac{F_{11} \lambda_{12} - F_{12} \lambda_{11}}{J^{c^{1/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (36)$$

$$F_{22}^{el} = -\frac{F_{21} \lambda_{12} - F_{22} \lambda_{11}}{J^{c^{1/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (37)$$

$$F_{33}^{el} = \frac{1}{J^{c^{1/3}} \lambda_{33}} \quad (38)$$

$$E_{11}^{el} = \frac{F_{11}^{el^2}}{2} + \frac{F_{21}^{el^2}}{2} - \frac{1}{2} \quad (39)$$

$$E_{21}^{el} = \frac{F_{11}^{el} F_{12}^{el}}{2} + \frac{F_{21}^{el} F_{22}^{el}}{2} \quad (40)$$

$$E_{12}^{el} = \frac{F_{11}^{el} F_{12}^{el}}{2} + \frac{F_{21}^{el} F_{22}^{el}}{2} \quad (41)$$

$$E_{22}^{el} = \frac{F_{12}^{el^2}}{2} + \frac{F_{22}^{el^2}}{2} - \frac{1}{2} \quad (42)$$

$$E_{33}^{el} = \frac{F_{33}^{el^2}}{2} - \frac{1}{2} \quad (43)$$

$$\tilde{S}_{11}^{el} = J^c \left(2 E_{11}^{el} \tilde{\mu}_{si} + \tilde{\lambda}_{si} (E_{11}^{el} + E_{22}^{el} + E_{33}^{el}) \right) \quad (44)$$

$$\tilde{S}_{21}^{el} = 2 E_{21}^{el} J^c \tilde{\mu}_{si} \quad (45)$$

$$\tilde{S}_{12}^{el} = 2 E_{12}^{el} J^c \tilde{\mu}_{si} \quad (46)$$

$$\tilde{S}_{22}^{el} = J^c \left(2 E_{22}^{el} \tilde{\mu}_{si} + \tilde{\lambda}_{si} (E_{11}^{el} + E_{22}^{el} + E_{33}^{el}) \right) \quad (47)$$

$$\tilde{S}_{33}^{el} = J^c \left(2 E_{33}^{el} \tilde{\mu}_{si} + \tilde{\lambda}_{si} (E_{11}^{el} + E_{22}^{el} + E_{33}^{el}) \right) \quad (48)$$

$$\tilde{S}_{11} = \frac{\tilde{S}_{11}^{\text{el}} \lambda_{22}^2 + \tilde{S}_{22}^{\text{el}} \lambda_{12}^2 - \tilde{S}_{12}^{\text{el}} \lambda_{12} \lambda_{22} - \tilde{S}_{21}^{\text{el}} \lambda_{12} \lambda_{22}}{Jc^{2/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (49)$$

$$\tilde{S}_{21} = \frac{\tilde{S}_{12}^{\text{el}} \lambda_{12} \lambda_{21} - \tilde{S}_{22}^{\text{el}} \lambda_{11} \lambda_{12} - \tilde{S}_{11}^{\text{el}} \lambda_{21} \lambda_{22} + \tilde{S}_{21}^{\text{el}} \lambda_{11} \lambda_{22}}{Jc^{2/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (50)$$

$$\tilde{S}_{12} = \frac{\tilde{S}_{12}^{\text{el}} \lambda_{11} \lambda_{22} - \tilde{S}_{22}^{\text{el}} \lambda_{11} \lambda_{12} - \tilde{S}_{11}^{\text{el}} \lambda_{21} \lambda_{22} + \tilde{S}_{21}^{\text{el}} \lambda_{12} \lambda_{21}}{Jc^{2/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (51)$$

$$\tilde{S}_{22} = \frac{\tilde{S}_{11}^{\text{el}} \lambda_{21}^2 + \tilde{S}_{22}^{\text{el}} \lambda_{11}^2 - \tilde{S}_{12}^{\text{el}} \lambda_{11} \lambda_{21} - \tilde{S}_{21}^{\text{el}} \lambda_{11} \lambda_{21}}{Jc^{2/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (52)$$

$$\tilde{S}_{33} = \frac{\tilde{S}_{33}^{\text{el}}}{Jc^{2/3} \lambda_{33}^2} \quad (53)$$

$$\tilde{P}_{11} = F_{11} \tilde{S}_{11} + F_{12} \tilde{S}_{21} \quad (54)$$

$$\tilde{P}_{21} = F_{21} \tilde{S}_{11} + F_{22} \tilde{S}_{21} \quad (55)$$

$$\tilde{P}_{12} = F_{11} \tilde{S}_{12} + F_{12} \tilde{S}_{22} \quad (56)$$

$$\tilde{P}_{22} = F_{21} \tilde{S}_{12} + F_{22} \tilde{S}_{22} \quad (57)$$

$$\tilde{P}_{33} = \tilde{S}_{33} \quad (58)$$

$$\tilde{\sigma}_{11} = \frac{F_{11} \tilde{P}_{11} + F_{12} \tilde{P}_{12}}{J} \quad (59)$$

$$\tilde{\sigma}_{21} = \frac{F_{11} \tilde{P}_{21} + F_{12} \tilde{P}_{22}}{J} \quad (60)$$

$$\tilde{\sigma}_{12} = \frac{F_{21} \tilde{P}_{11} + F_{22} \tilde{P}_{12}}{J} \quad (61)$$

$$\tilde{\sigma}_{22} = \frac{F_{21} \tilde{P}_{21} + F_{22} \tilde{P}_{22}}{J} \quad (62)$$

$$\tilde{\sigma}_{33} = \frac{\tilde{P}_{33}}{J} \quad (63)$$

$$\tilde{\tau}_{11} = \frac{2\tilde{\sigma}_{11}}{3} - \frac{\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{33}}{3} \quad (64)$$

$$\tilde{\tau}_{21} = \tilde{\sigma}_{21} \quad (65)$$

$$\tilde{\tau}_{12} = \tilde{\sigma}_{12} \quad (66)$$

$$\tilde{\tau}_{22} = \frac{2\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{11}}{3} - \frac{\tilde{\sigma}_{33}}{3} \quad (67)$$

$$\tilde{\tau}_{33} = \frac{2\tilde{\sigma}_{33}}{3} - \frac{\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{11}}{3} \quad (68)$$

$$\tilde{\sigma}_{\text{eff}} = \sqrt{\frac{3}{2}(\tilde{\tau}_{11}^2 + \tilde{\tau}_{22}^2 + \tilde{\tau}_{33}^2 + 2\tilde{\tau}_{12}^2)} \quad (69)$$

$$\tilde{M}_{11}^{\text{el}} = -\frac{J(F_{11}^{\text{el}} F_{12}^{\text{el}} \tilde{\tau}_{12} - F_{11}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{11} + F_{12}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{22} - F_{21}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{21})}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (70)$$

$$\tilde{M}_{21}^{\text{el}} = -\frac{J(F_{12}^{\text{el}^2} \tilde{\tau}_{12} - F_{22}^{\text{el}^2} \tilde{\tau}_{21} - F_{12}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{11} + F_{12}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{22})}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (71)$$

$$\tilde{M}_{12}^{\text{el}} = \frac{J(F_{11}^{\text{el}^2} \tilde{\tau}_{12} - F_{21}^{\text{el}^2} \tilde{\tau}_{21} - F_{11}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{11} + F_{11}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{22})}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (72)$$

$$\tilde{M}_{22}^{\text{el}} = \frac{J(F_{11}^{\text{el}} F_{12}^{\text{el}} \tilde{\tau}_{12} - F_{12}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{11} + F_{11}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{22} - F_{21}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{21})}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (73)$$

$$\tilde{M}_{33}^{\text{el}} = J \tilde{\tau}_{33} \quad (74)$$

Viscoplastic rates:

$$\dot{F}_{11}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{11}^{\text{el}} \lambda_{11}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{12}^{\text{el}} \lambda_{21}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \quad (75)$$

$$\dot{F}_{21}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{21}^{\text{el}} \lambda_{11}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{22}^{\text{el}} \lambda_{21}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \quad (76)$$

$$\dot{F}_{12}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{11}^{\text{el}} \lambda_{12}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{12}^{\text{el}} \lambda_{22}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \quad (77)$$

$$\dot{F}_{22}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{21}^{\text{el}} \lambda_{12}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{22}^{\text{el}} \lambda_{22}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \quad (78)$$

$$\dot{F}_{33}^{\text{p}} = \frac{3 \tilde{M}_{33}^{\text{el}} \dot{d}_0 \lambda_{33} \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m}{2 J \tilde{\sigma}_{\text{eff}}} \quad (79)$$

Viscoplastic rate equations in non-dimensional form:

$$\frac{d\lambda_{xx}}{dt} = \frac{1}{t_{\text{ref}}} \frac{d\lambda_{xx}}{d\tilde{t}} = \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\text{eff}}} (\tilde{M}_{11}^{\text{el}} \lambda_{xx} + \tilde{M}_{12}^{\text{el}} \lambda_{yx}) \text{H}\left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1\right)^m \quad (80)$$

$$\frac{d\lambda_{xx}}{d\tilde{t}} = \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\text{eff}}} (\tilde{M}_{11}^{\text{el}} \lambda_{xx} + \tilde{M}_{12}^{\text{el}} \lambda_{yx}) \text{H}\left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1\right)^m \quad (81)$$

$$\text{where, } \dot{d}_0 = \dot{d}_0 t_{\text{ref}} \quad (82)$$

Stress equilibrium Equation:

$$\nabla_{\mathbf{X}} \cdot \mathbf{P} = \mathbf{0}. \quad (83)$$

$$\frac{\partial P_{11}}{\partial X} + \frac{\partial P_{12}}{\partial Y} = 0 \quad (84)$$

$$\text{and, } \frac{\partial P_{21}}{\partial X} + \frac{\partial P_{22}}{\partial Y} = 0 \quad (85)$$

In non-dimensional form:

$$\frac{E_0}{H} \frac{\partial \tilde{P}_{11}}{\partial \tilde{X}} + \frac{E_0}{H} \frac{\partial \tilde{P}_{12}}{\partial \tilde{Y}} = 0 \quad (86)$$

$$\text{and, } \frac{E_0}{H} \frac{\partial \tilde{P}_{21}}{\partial \tilde{X}} + \frac{E_0}{H} \frac{\partial \tilde{P}_{22}}{\partial \tilde{Y}} = 0 \quad (87)$$

So,

$$\frac{\partial \tilde{P}_{11}}{\partial \tilde{X}} + \frac{\partial \tilde{P}_{12}}{\partial \tilde{Y}} = 0 \quad (88)$$

$$\text{and, } \frac{\partial \tilde{P}_{21}}{\partial \tilde{X}} + \frac{\partial \tilde{P}_{22}}{\partial \tilde{Y}} = 0 \quad (89)$$

Mass conservation Equation:

$$\frac{\partial c}{\partial t} = -\nabla_{\mathbf{X}} \cdot \mathbf{j} = -\left(\frac{\partial j_x}{\partial X} + \frac{\partial j_y}{\partial Y}\right) \quad (90)$$

For one way coupling:

$$\mathbf{j} = -D_0 \nabla_{\mathbf{X}} c \quad (91)$$

$$\tilde{j}_x = j_x H / (c_{\max} D_0) \quad (92)$$

$$= -D_0 \frac{\partial c}{\partial X} H / (c_{\max} D_0) \quad (93)$$

$$= -\frac{\partial \tilde{c}}{\partial \tilde{X}} \quad (94)$$

$$\tilde{j}_y = j_y H / (c_{\max} D_0) \quad (95)$$

$$= -\frac{\partial \tilde{c}}{\partial \tilde{Y}} \quad (96)$$

For two way coupling:

$$\mathbf{j} = -\frac{1}{R_g T} \frac{D\chi_{\max}\tilde{c}}{V_m^b} (F)^{-1} (F)^{-\top} \nabla_{\mathbf{X}} \mu \quad (97)$$

$$D = D_0 \exp\left(\frac{\alpha S_h}{E_0}\right) \quad (98)$$

$$\mu = \mu_0 + \mu_s \quad (99)$$

$$\mu_0 = R_g T \log(\gamma \tilde{c}) \quad (100)$$

$$\gamma = \frac{1}{1 - \tilde{c}} \exp\left(\frac{1}{R_g T} [2(A_0 - 2B_0)\tilde{c} - 3(A_0 - B_0)(\tilde{c}^2)]\right) \quad (101)$$

$$\mu_s = \frac{V_m^b}{\chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} C_{mnkl} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} (J^c \frac{\partial C_{ijkl}}{\partial \tilde{c}} + \frac{\partial J^c}{\partial \tilde{c}} C_{ijkl}) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (102)$$

$$= (\mu_1 + \mu_2 + \mu_3) / \chi_{\max} \quad (103)$$

$$\tilde{\mu} = \tilde{\mu}_0 + (\tilde{\mu}_1 + \tilde{\mu}_2 + \tilde{\mu}_3) / \chi_{\max} \quad (104)$$

$$\tilde{\mu}_0 = \log(\gamma \tilde{c}) \quad (105)$$

$$\tilde{\mu}_1 = -\frac{1}{6(J^c)} \frac{\partial J^c}{\partial \tilde{c}} [\tilde{S}_{11}^{\text{el}} \tilde{E}_{11}^{\text{el}} + \tilde{S}_{22}^{\text{el}} \tilde{E}_{22}^{\text{el}} + 2\tilde{S}_{12}^{\text{el}} \tilde{E}_{12}^{\text{el}} + \tilde{S}_{33}^{\text{el}} \tilde{E}_{33}^{\text{el}}] \quad (106)$$

$$\tilde{\mu}_2 = -\frac{1}{3(J^c)} \frac{\partial J^c}{\partial \tilde{c}} [\tilde{S}_{11}^{\text{el}} + \tilde{S}_{22}^{\text{el}} + \tilde{S}_{33}^{\text{el}}] \quad (107)$$

$$\tilde{\mu}_3 = \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}} \quad (108)$$

$$= \frac{1}{2} J^c [2\tilde{\mu}'_{\text{si}}(\tilde{c}) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{ij}^{\text{el}} + \tilde{\lambda}'_{\text{si}}(\tilde{c}) (\tilde{E}_{11}^{\text{el}} + \tilde{E}_{22}^{\text{el}} + \tilde{E}_{33}^{\text{el}}) \tilde{E}_{ij}^{\text{el}} \delta_{ij}] \quad (109)$$

$$= \frac{1}{2} J^c [2\tilde{\mu}'_{\text{si}}(\tilde{c}) ((\tilde{E}_{11}^{\text{el}})^2 + (\tilde{E}_{22}^{\text{el}})^2 + (\tilde{E}_{33}^{\text{el}})^2 + 2(\tilde{E}_{12}^{\text{el}})^2) + \tilde{\lambda}'_{\text{si}}(\tilde{c}) (\tilde{E}_{11}^{\text{el}} + \tilde{E}_{22}^{\text{el}} + \tilde{E}_{33}^{\text{el}})^2] \quad (110)$$

$$\mathbf{j} = -\frac{D\chi_{\max}\tilde{c}}{V_m^b} \tilde{\mathbf{F}}^{-1} (\tilde{\mathbf{F}}^{-1})^\top \nabla_{\mathbf{X}} \tilde{\mu} \quad (111)$$

$$\tilde{\mathbf{j}} = \mathbf{j} H V_m^b / (\chi_{\max} D_0) \quad (112)$$

$$= -\frac{D}{D_0} H \tilde{c} \tilde{\mathbf{F}}^{-1} (\tilde{\mathbf{F}}^{-1})^\top \nabla_{\mathbf{X}} \tilde{\mu} \quad (113)$$

$$\tilde{j}_x = \frac{-\bar{D} H \tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial \tilde{X}} (\tilde{F}_{12}^2 + \tilde{F}_{22}^2) - \frac{\partial \tilde{\mu}}{\partial \tilde{Y}} (\tilde{F}_{11} \tilde{F}_{12} + \tilde{F}_{21} \tilde{F}_{22}) \right) \quad (114)$$

$$= \frac{-\bar{D} \tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial \tilde{X}} (\tilde{F}_{12}^2 + \tilde{F}_{22}^2) - \frac{\partial \tilde{\mu}}{\partial \tilde{Y}} (\tilde{F}_{11} \tilde{F}_{12} + \tilde{F}_{21} \tilde{F}_{22}) \right) \quad (115)$$

$$\tilde{j}_y = \frac{-\bar{D} H \tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial \tilde{Y}} (\tilde{F}_{11}^2 + \tilde{F}_{21}^2) - \frac{\partial \tilde{\mu}}{\partial \tilde{X}} (\tilde{F}_{11} \tilde{F}_{12} + \tilde{F}_{21} \tilde{F}_{22}) \right) \quad (116)$$

$$= \frac{-\bar{D} \tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial \tilde{Y}} (\tilde{F}_{11}^2 + \tilde{F}_{21}^2) - \frac{\partial \tilde{\mu}}{\partial \tilde{X}} (\tilde{F}_{11} \tilde{F}_{12} + \tilde{F}_{21} \tilde{F}_{22}) \right) \quad (117)$$

$$(118)$$

In non-dimensional form:

$$c_{\max} \frac{D_0}{H^2} \frac{\partial \tilde{c}}{\partial \tilde{t}} = - \left(\frac{1}{H} \frac{\partial \tilde{j}_x}{\partial \tilde{X}} + \frac{1}{H} \frac{\partial \tilde{j}_y}{\partial \tilde{Y}} \right) c_{\max} \frac{D_0}{H} \quad (119)$$

$$\text{so, } \frac{\partial \tilde{c}}{\partial \tilde{t}} = - \left(\frac{\partial \tilde{j}_x}{\partial \tilde{X}} + \frac{\partial \tilde{j}_y}{\partial \tilde{Y}} \right) \quad (120)$$

Secondary Variables (in DIS+SED) for the expression of flux in two-way coupling:

$$\tilde{\mathbf{F}}_X = \frac{\partial \tilde{\mathbf{F}}}{\partial \tilde{X}} = \begin{bmatrix} \frac{\partial^2 \tilde{u}}{\partial \tilde{X}^2} & \frac{\partial^2 \tilde{u}}{\partial \tilde{X} \tilde{Y}} & 0 \\ \frac{\partial^2 \tilde{v}}{\partial \tilde{X}^2} & \frac{\partial^2 \tilde{v}}{\partial \tilde{X} \tilde{Y}} & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (121)$$

$$\tilde{\mathbf{F}}_Y = \frac{\partial \tilde{\mathbf{F}}}{\partial \tilde{Y}} = \begin{bmatrix} \frac{\partial^2 \tilde{u}}{\partial \tilde{X} \tilde{Y}} & \frac{\partial^2 \tilde{u}}{\partial \tilde{Y}^2} & 0 \\ \frac{\partial^2 \tilde{v}}{\partial \tilde{X} \tilde{Y}} & \frac{\partial^2 \tilde{v}}{\partial \tilde{Y}^2} & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (122)$$

$$\tilde{F}_{11_x}^{\text{el}} = -\frac{1}{3} (J^c)^{-4/3} \frac{dJ^c}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} F_{11} + (J^c)^{-1/3} F_{11_x} \quad (123)$$

$$\tilde{F}_{12_x}^{\text{el}} = -\frac{1}{3} (J^c)^{-4/3} \frac{dJ^c}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} F_{12} + (J^c)^{-1/3} F_{12_x} \quad (124)$$

$$\tilde{F}_{21_x}^{\text{el}} = -\frac{1}{3} (J^c)^{-4/3} \frac{dJ^c}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} F_{21} + (J^c)^{-1/3} F_{21_x} \quad (125)$$

$$\tilde{F}_{22_x}^{\text{el}} = -\frac{1}{3} (J^c)^{-4/3} \frac{dJ^c}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} F_{22} + (J^c)^{-1/3} F_{22_x} \quad (126)$$

$$\tilde{F}_{33_x}^{\text{el}} = \quad (127)$$

$$\tilde{E}_{11_x}^{\text{el}} = \tilde{F}_{11}^{\text{el}} \tilde{F}_{11_x}^{\text{el}} + \tilde{F}_{21}^{\text{el}} \tilde{F}_{21_x}^{\text{el}} \quad (128)$$

$$\tilde{E}_{22_x}^{\text{el}} = \tilde{F}_{12}^{\text{el}} \tilde{F}_{12_x}^{\text{el}} + \tilde{F}_{22}^{\text{el}} \tilde{F}_{22_x}^{\text{el}} \quad (129)$$

$$\tilde{E}_{12_x}^{\text{el}} = 0.5 [\tilde{F}_{11_x}^{\text{el}} \tilde{F}_{12}^{\text{el}} + \tilde{F}_{11}^{\text{el}} \tilde{F}_{12_x}^{\text{el}} + \tilde{F}_{21_x}^{\text{el}} \tilde{F}_{22}^{\text{el}} + \tilde{F}_{21}^{\text{el}} \tilde{F}_{22_x}^{\text{el}}] = \tilde{E}_{21_x}^{\text{el}} \quad (130)$$

$$\tilde{E}_{33_x}^{\text{el}} = \quad (131)$$

$$\tilde{E}_{\text{trace}}^{\text{el}} = \tilde{E}_{11}^{\text{el}} + \tilde{E}_{22}^{\text{el}} + \tilde{E}_{33}^{\text{el}} \quad (132)$$

$$\tilde{E}_{\text{trace}_x}^{\text{el}} = \tilde{E}_{11_x}^{\text{el}} + \tilde{E}_{22_x}^{\text{el}} + \tilde{E}_{33_x}^{\text{el}} \quad (133)$$

$$\tilde{S}_{11_x}^{\text{el}} = \frac{dJ^c}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \frac{\tilde{S}_{11}^{\text{el}}}{J^c} + J^c \left(2 \frac{d\tilde{\mu}_{si}}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \tilde{E}_{11}^{\text{el}} + 2\tilde{\mu}_{si} \tilde{E}_{11_x}^{\text{el}} + \frac{d\tilde{\lambda}_{si}}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \tilde{E}_{\text{trace}}^{\text{el}} + \tilde{\lambda}_{si} \tilde{E}_{\text{trace}_x}^{\text{el}} \right) \quad (134)$$

$$\tilde{S}_{22_x}^{\text{el}} = \frac{dJ^c}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \frac{\tilde{S}_{22}^{\text{el}}}{J^c} + J^c \left(2 \frac{d\tilde{\mu}_{si}}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \tilde{E}_{22}^{\text{el}} + 2\tilde{\mu}_{si} \tilde{E}_{22_x}^{\text{el}} + \frac{d\tilde{\lambda}_{si}}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \tilde{E}_{\text{trace}}^{\text{el}} + \tilde{\lambda}_{si} \tilde{E}_{\text{trace}_x}^{\text{el}} \right) \quad (135)$$

$$\tilde{S}_{33_x}^{\text{el}} = \frac{dJ^c}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \frac{\tilde{S}_{33}^{\text{el}}}{J^c} + J^c \left(2 \frac{d\tilde{\mu}_{si}}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \tilde{E}_{33}^{\text{el}} + 2\tilde{\mu}_{si} \tilde{E}_{33_x}^{\text{el}} + \frac{d\tilde{\lambda}_{si}}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \tilde{E}_{\text{trace}}^{\text{el}} + \tilde{\lambda}_{si} \tilde{E}_{\text{trace}_x}^{\text{el}} \right) \quad (136)$$

$$\tilde{S}_{12_x}^{\text{el}} = 2 \frac{dJ^c}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \tilde{\mu}_{si} \tilde{E}_{12}^{\text{el}} + 2J^c \frac{d\tilde{\mu}_{si}}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \tilde{E}_{12}^{\text{el}} + 2J^c \tilde{\mu}_{si} \tilde{E}_{12_x}^{\text{el}} = \tilde{S}_{21_x}^{\text{el}} \quad (137)$$

$$\gamma = \frac{1}{1-\tilde{c}} \exp\left(\frac{1}{R_g T} [2(A_0 - 2B_0)\tilde{c} - 3(A_0 - B_0)(\tilde{c}^2)]\right) \quad (138)$$

$$\frac{\partial \gamma}{\partial \tilde{X}} = \gamma_x = \frac{1}{(1-\tilde{c})^2} \frac{\partial \tilde{c}}{\partial \tilde{X}} \exp(\dots) + \frac{1}{1-\tilde{c}} \exp(\dots) \frac{1}{R_g T} [2(A_0 - 2B_0) \frac{\partial \tilde{c}}{\partial \tilde{X}} - 3(A_0 - B_0)(2\tilde{c} \frac{\partial \tilde{c}}{\partial \tilde{X}})] \quad (139)$$

$$= \frac{1}{1-\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \gamma + \frac{\gamma}{R_g T} [2(A_0 - 2B_0) \frac{\partial \tilde{c}}{\partial \tilde{X}} - 3(A_0 - B_0)(2\tilde{c} \frac{\partial \tilde{c}}{\partial \tilde{X}})] \quad (140)$$

$$(141)$$

$$\tilde{\mu}_0 = \log(\gamma \tilde{c}) \quad (142)$$

$$\tilde{\mu}_{0_x} = \frac{1}{\gamma} \gamma_x + \frac{1}{\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \quad (143)$$

$$\tilde{\mu}_1 = -\frac{1}{6(J^c)} \frac{\partial J^c}{\partial \tilde{c}} [\tilde{S}_{11}^{\text{el}} \tilde{E}_{11}^{\text{el}} + \tilde{S}_{22}^{\text{el}} \tilde{E}_{22}^{\text{el}} + 2\tilde{S}_{12}^{\text{el}} \tilde{E}_{12}^{\text{el}} + \tilde{S}_{33}^{\text{el}} \tilde{E}_{33}^{\text{el}}] \quad (144)$$

$$= -\frac{1}{2J^c} \eta \chi_{\text{max}} [\tilde{S}_{11}^{\text{el}} \tilde{E}_{11}^{\text{el}} + \tilde{S}_{22}^{\text{el}} \tilde{E}_{22}^{\text{el}} + 2\tilde{S}_{12}^{\text{el}} \tilde{E}_{12}^{\text{el}} + \tilde{S}_{33}^{\text{el}} \tilde{E}_{33}^{\text{el}}] \quad (145)$$

$$\tilde{\mu}_{1_x} = (-\frac{1}{2} \eta \chi_{\text{max}}) * (-\frac{1}{J^c} 3\eta \chi_{\text{max}}) * \frac{\partial \tilde{c}}{\partial \tilde{X}} [\dots] - \frac{1}{2J^c} \eta \chi_{\text{max}} [\dots]_x \quad (146)$$

$$= -3\eta \chi_{\text{max}} \frac{1}{J^c} \frac{\partial \tilde{c}}{\partial \tilde{X}} \tilde{\mu}_1 - \eta \chi_{\text{max}} \frac{1}{2J^c} [\tilde{S}_{11_x}^{\text{el}} \tilde{E}_{11}^{\text{el}} + \tilde{S}_{11}^{\text{el}} \tilde{E}_{11_x}^{\text{el}} + \tilde{S}_{22_x}^{\text{el}} \tilde{E}_{22}^{\text{el}} + \tilde{S}_{22}^{\text{el}} \tilde{E}_{22_x}^{\text{el}} \quad (147)$$

$$+ \tilde{S}_{33_x}^{\text{el}} \tilde{E}_{33}^{\text{el}} + \tilde{S}_{33}^{\text{el}} \tilde{E}_{33_x}^{\text{el}} + 2\tilde{S}_{12_x}^{\text{el}} \tilde{E}_{12}^{\text{el}} + 2\tilde{S}_{12}^{\text{el}} \tilde{E}_{12_x}^{\text{el}}] \quad (148)$$

$$\tilde{\mu}_2 = -\frac{1}{3(J^c)} \frac{\partial J^c}{\partial \tilde{c}} [\tilde{S}_{11}^{\text{el}} + \tilde{S}_{22}^{\text{el}} + \tilde{S}_{33}^{\text{el}}] \quad (149)$$

$$= -\frac{1}{J^c} \eta \chi_{\text{max}} [\tilde{S}_{11}^{\text{el}} + \tilde{S}_{22}^{\text{el}} + \tilde{S}_{33}^{\text{el}}] \quad (150)$$

$$\tilde{\mu}_{2_x} = -\frac{3\eta \chi_{\text{max}}}{J^c} \frac{\partial \tilde{c}}{\partial \tilde{X}} \tilde{\mu}_2 - \frac{\eta \chi_{\text{max}}}{J^c} [\tilde{S}_{11_x}^{\text{el}} + \tilde{S}_{22_x}^{\text{el}} + \tilde{S}_{33_x}^{\text{el}}] \quad (151)$$

$$\tilde{\mu}_3 = \frac{1}{2} J^c [2\tilde{\mu}'_{\text{si}}(\tilde{c})((\tilde{E}_{11}^{\text{el}})^2 + (\tilde{E}_{22}^{\text{el}})^2 + (\tilde{E}_{33}^{\text{el}})^2 + 2(\tilde{E}_{12}^{\text{el}})^2) + \tilde{\lambda}'_{\text{si}}(c)(\tilde{E}_{11}^{\text{el}} + \tilde{E}_{22}^{\text{el}} + \tilde{E}_{33}^{\text{el}})^2] \quad (152)$$

$$\tilde{\mu}_{3_x} = \frac{dJ^c}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \frac{\tilde{\mu}_3}{J^c} + \frac{J^c}{2} \left[2\tilde{\mu}'_{\text{si}}(2\tilde{E}_{11}^{\text{el}}\tilde{E}_{11_x}^{\text{el}} + 2\tilde{E}_{22}^{\text{el}}\tilde{E}_{22_x}^{\text{el}} + 2\tilde{E}_{33}^{\text{el}}\tilde{E}_{33_x}^{\text{el}} + 4\tilde{E}_{12}^{\text{el}}\tilde{E}_{12_x}^{\text{el}}) + 2\tilde{\lambda}'_{\text{si}}(\tilde{E}_{\text{trace}}^{\text{el}}\tilde{E}_{\text{trace}_x}^{\text{el}}) \right] \quad (153)$$

$$\tilde{\mu}_x = \tilde{\mu}_{0_x} + (\tilde{\mu}_{1_x} + \tilde{\mu}_{2_x} + \tilde{\mu}_{3_x})/\chi_{\text{max}} \quad (154)$$

1.6 Boundary and Initial Conditions

$$\tilde{c}(\tilde{X}, \tilde{Y}, 0) = 0 \quad (155)$$

$$\tilde{u}(\tilde{X}, \tilde{Y}, 0) = 0 \quad (156)$$

$$\tilde{v}(\tilde{X}, \tilde{Y}, 0) = 0 \quad (157)$$

$$\tilde{u}(\tilde{X}, 0, \tilde{t}) = \tilde{v}(\tilde{X}, 0, \tilde{t}) = 0 \quad (158)$$

$$\tilde{u}(-1/2, \tilde{Y}, \tilde{t}) = \tilde{u}(1/2, \tilde{Y}, \tilde{t}) = 0 \quad (159)$$

$$\tilde{j}_x(\tilde{X}, 1, \tilde{t}) = \tilde{j}_0(1 - \tilde{c}(\tilde{X}, 1, \tilde{t})) \quad (160)$$