Research Paper

Himanshu Sharma

July 22, 2024

1 Introduction

introduction

2 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

$$Mel_{11} = -\frac{J\,\left(F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{12}\,\tau_{12} - F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{22}\,\tau_{11} + F^{\mathrm{el}}_{12}\,F^{\mathrm{el}}_{21}\,\tau_{22} - F^{\mathrm{el}}_{21}\,F^{\mathrm{el}}_{22}\,\tau_{21}\right)}{F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{22} - F^{\mathrm{el}}_{12}\,F^{\mathrm{el}}_{21}} \tag{1}$$

$$Mel_{21} = -\frac{J\,\left({F^{\mathrm{el}}_{12}}^2\,\tau_{12} - {F^{\mathrm{el}}_{22}}^2\,\tau_{21} - F^{\mathrm{el}}_{12}\,F^{\mathrm{el}}_{22}\,\tau_{11} + F^{\mathrm{el}}_{12}\,F^{\mathrm{el}}_{22}\,\tau_{22}\right)}{F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{22} - F^{\mathrm{el}}_{12}\,F^{\mathrm{el}}_{21}} \tag{2}$$

$$Mel_{12} = \frac{J\,\left({F^{\mathrm{el}}_{11}}^2\,\tau_{12} - {F^{\mathrm{el}}_{21}}^2\,\tau_{21} - F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{21}\,\tau_{11} + F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{21}\,\tau_{22}\right)}{F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{22} - F^{\mathrm{el}}_{12}\,F^{\mathrm{el}}_{21}} \tag{3}$$

$$Mel_{22} = \frac{J\,\left(F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{12}\,\tau_{12} - F^{\mathrm{el}}_{12}\,F^{\mathrm{el}}_{21}\,\tau_{11} + F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{22}\,\tau_{22} - F^{\mathrm{el}}_{21}\,F^{\mathrm{el}}_{22}\,\tau_{21}\right)}{F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{22} - F^{\mathrm{el}}_{12}\,F^{\mathrm{el}}_{21}} \tag{4}$$

$$Mel_{33} = J\,\tau_{33} \tag{5}$$

$$\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{X}, t) \tag{6}$$

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

$$\boldsymbol{u}(\boldsymbol{X}, t) = \boldsymbol{x}(\boldsymbol{X}, t) - \boldsymbol{X} = [u(\boldsymbol{X}, t), v(\boldsymbol{X}, t), w(\boldsymbol{X}, t)]^{\mathsf{T}} \tag{7}$$

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

$$\mathbf{F} = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} = \boldsymbol{\nabla}_{\boldsymbol{X}} \boldsymbol{u} + \mathbf{I} \tag{8}$$

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^{\mathsf{T}}\mathbf{F} - \mathbf{I}) \tag{9}$$

Assuming plane strain deformation,

$$\mathbf{F} = \begin{bmatrix} 1 + \frac{\partial u}{\partial X} & \frac{\partial u}{\partial Y} & 0 \\ \frac{\partial v}{\partial X} & 1 + \frac{\partial v}{\partial \partial Y} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} F_{11} & F_{12} & 0 \\ F_{21} & F_{22} & 0 \\ 0 & 0 & F_{33} \end{bmatrix} \tag{10}$$

Decomposition of deformation gradient

$$\mathbf{F} = \mathbf{F}^{\mathrm{el}}\mathbf{F}^{\mathrm{inel}} \tag{11}$$

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

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

$$\mathbf{F}^{\mathrm{inel}} = \mathbf{F}^{\mathrm{c}}\mathbf{F}^{\mathrm{p}} \tag{12}$$

2.1 Viscoplastic Deformation

$$\dot{\mathbf{F}}^{\mathrm{p}} = (J)^{-1}\frac{3}{2}\frac{\mathbf{M}_{\mathbf{0}}^{\mathrm{el}}\mathbf{F}^{\mathrm{p}}}{\sigma_{\mathrm{eff}}}\dot{d}_0\langle\frac{\sigma_{\mathrm{eff}}}{\sigma_{\mathrm{f}}} - 1\rangle^{\mathrm{m}} \tag{13}$$

$$\mathbf{M}_{\mathbf{0}}^{\mathrm{el}} = J(\mathbf{F}^{\mathrm{el}})^{\mathsf{T}}\boldsymbol{\tau}(\mathbf{F}^{\mathrm{el}})^{-\mathsf{T}} \tag{14}$$

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

$$\mathbf{F}^{\mathrm{p}} = \begin{bmatrix} \lambda_{xx} & \lambda_{xy} & 0 \\ \lambda_{yx} & \lambda_{yy} & 0 \\ 0 & 0 & \lambda_{zz} \end{bmatrix} \tag{15}$$

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

$$\lambda_{zz} = 1/(\lambda_{xx}\lambda_{yy} - \lambda_{xy}\lambda_{yx}) \tag{16}$$

2.2 Deformation due to concentration gradient

$$\mathbf{F}^{\mathrm{c}} = (J^c)^{1/3}\mathbf{I} \tag{17}$$

$$\text{where } J^c = 1 + 3\eta\chi_{\max}\tilde{c} \tag{18}$$

$$\mathbf{F}^{\mathrm{inel}} = \mathbf{F}^{\mathrm{p}}\mathbf{F}^{\mathrm{c}} \tag{19}$$

$$\mathbf{F}^{\mathrm{el}} = \mathbf{F}((\mathbf{F}^{\mathrm{p}}\mathbf{F}^{\mathrm{c}}))^{-1} \tag{20}$$

$$\mathbf{E}^{\mathrm{el}} = \frac{1}{2}\left[(\mathbf{F}^{\mathrm{el}})^{\mathsf{T}}\mathbf{F}^{\mathrm{el}} - \mathbf{I}\right] \tag{21}$$

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

$$W(\mathbf{F}, c) = \frac{J^c}{2}\frac{E(c)}{1+\nu}\left(\frac{\nu}{1-2\nu}(\mathrm{tr}\mathbf{E}^{\mathrm{el}})^2 + \mathrm{tr}(\mathbf{E}^{\mathrm{el}}\mathbf{E}^{\mathrm{el}})\right) \tag{22}$$

$$\mathbf{S}^{\mathrm{el}} = J^c(2\mu_{\mathrm{si}}(c)\mathbf{E}^{\mathrm{el}} + \lambda_{\mathrm{si}}(c)\mathrm{tr}(\mathbf{E}^{\mathrm{el}})\mathbf{I}) \tag{23}$$

$$\mathbf{S} = (\mathbf{F}^{\mathrm{c}})^{-1}(\mathbf{F}^{\mathrm{p}})^{-1}\mathbf{S}^{\mathrm{el}}(\mathbf{F}^{\mathrm{p}})^{-\mathsf{T}}(\mathbf{F}^{\mathrm{c}})^{-\mathsf{T}} \tag{24}$$

$$\mathbf{P} = \mathbf{F}\mathbf{S} \tag{25}$$
$$\tag{26}$$

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

$$\boldsymbol{\sigma} = (J)^{-1}\mathbf{P}\mathbf{F}^{\mathsf{T}} \tag{27}$$
$$\text{where, } J = \det(\mathbf{F}) \tag{28}$$

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

$$\boldsymbol{\tau} = \boldsymbol{\sigma} - (1/3)\mathrm{tr}(\boldsymbol{\sigma})\mathbf{I} \tag{29}$$
$$\tag{30}$$

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

$$\sigma_{\text{eff}} = \sqrt{\frac{3}{2}(\tau_{11}^2 + \tau_{22}^2 + \tau_{33}^2 + 2 + \tau_{12}^2)} \tag{31}$$

2.3 CZM Equations in Deepro's thesis

$$\Delta = \sqrt{\Delta_n^2 + \Delta_t^2} \tag{32}$$
$$T_n = K_n(1-d)\langle \Delta_n \rangle \tag{33}$$
$$T_t = K_t(1-d)\Delta_t \tag{34}$$
$$d = \begin{cases} 0 & \text{if } \Delta < \delta_{e,c} \\ \frac{\delta e}{\Delta}\left(\frac{\Delta - \delta_{e,c}}{\delta e - \delta_{e,c}}\right) & \text{if } \delta_{e,c} < \Delta < \delta e \\ 1 & \text{if } \Delta > \delta_e \end{cases} \tag{35}$$
$$\delta_e \neq \sqrt{\left(\frac{2G_n}{\sigma_{\max}}\right)^2 + \left(\frac{2G_t}{\tau_{\max}}\right)^2} \tag{36}$$
$$\delta_{e,c} \neq \sqrt{\left(\frac{\sigma_{max}}{K_n}\right)^2 + \left(\frac{\tau_{max}}{K_t}\right)^2} \tag{37}$$
$$\tag{38}$$

2.4 CZM Equations in COMSOL

$$\boldsymbol{u} = \{0, 0, \langle g_n \rangle\} + \mathbf{T}_b^{-\mathsf{T}} \cdot \Delta \boldsymbol{g}_t \tag{39}$$

$$u_m = \|\boldsymbol{u}\| \tag{40}$$

$$u_{\text{m, max}} = \max(u_m, u_{\text{m, max}}^{\text{old}}) \text{ - same over the boundary or varies locally?} \tag{41}$$

$$\boldsymbol{f} = \boldsymbol{k}\boldsymbol{u}(1-d) \text{ ; Nominal traction} \tag{42}$$

$$u_{0\text{t}} = \frac{\sigma_{0t}}{k_{\text{n}}} \tag{43}$$

$$u_{0\text{s}} = \frac{\sigma_{0s}}{k_{\text{t}}} \tag{44}$$

$$u_{0\text{m}} = u_{0\text{t}} u_{0\text{s}} \sqrt{\frac{{u_m}^2}{\langle u_{\text{I}} \rangle^2 u_{0\text{s}}^2 + u_{\text{II}}^2 u_{0\text{t}}^2}} \text{ - why does it contain time varying quantities?} \tag{45}$$

$$\beta = \frac{u_{\text{II}}}{u_{\text{I}}} \text{ - constant ?} \tag{46}$$

$$u_{\text{mf}} = \begin{cases} \frac{2(1+\beta^2)}{u_{0\text{m}}} \left[\left(\frac{k_n}{G_{ct}} \right)^{\alpha} + \left(\frac{\beta^2 k_t}{G_{cs}} \right)^{\alpha} \right]^{-\frac{1}{\alpha}} & \text{if } u_{\text{I}} > 0 \\ \frac{2G_{\text{cs}}}{\sigma_s} & \text{if } u_{\text{I}} < 0 \end{cases} \tag{47}$$

$$\tag{48}$$

2.4.1 variable names in COMSOL

Variables in Decohesion node

$$u0t = \frac{\sigma_t}{k_n}, \text{ Damage initiation displacement, tension} \tag{49}$$

$$u0s = \frac{\sigma_s}{k_{teq}}, \text{ Damage initiation displacement, Shear} \tag{50}$$

$$u0m_{ap1} = \text{ Damage initiation displacement, Mixed Mode} \tag{51}$$

$$uft = \frac{2G_{ct}}{\sigma_t}, \text{ Failure displacement, tension} \tag{52}$$

$$ufs = \frac{2G_{cs}}{\sigma_s}, \text{ Failure displacement, Shear} \tag{53}$$

$$ufm_{ap1} = \text{ Failure displacement, Mixed Mode} \tag{54}$$

$$u_{I_{ap1}} = \text{ Mode I displacement jump} \tag{55}$$

$$u_{II_{ap1}} = \text{ Mode II displacement jump} \tag{56}$$

$$dmg_{ap1} = dmg = \text{Damage} \tag{57}$$

$$dmg_{ratio_{ap1}} = \frac{um_{max_{ap1}} - u0m_{ap1}}{ufm_{ap1} - u0m_{ap1}}, \text{ Damage evolution ratio} \tag{58}$$

Stress equilibrium equation:

$$\boldsymbol{\nabla}_{\boldsymbol{X}} \cdot \mathbf{P} = 0. \tag{59}$$

Mass conservation equation:

$$\frac{\partial c}{\partial t} = -\boldsymbol{\nabla}_{\boldsymbol{X}} \cdot \boldsymbol{j} \tag{60}$$

2.5 Non-Dimensionalization

$$\begin{aligned}
\tilde{c} &= c/c_{\max} & \tilde{\boldsymbol{j}} &= \boldsymbol{j}H/(c_{\max}D_0) \\
\text{where, } c_{\max} &= \chi_{\max}/V_m^B & & \\
\tilde{u} &= u/H & \tilde{v} &= v/H \\
\tilde{X} &= X/H & \tilde{Y} &= Y/H \\
\tilde{t} &= D_0 t/H^2 & \tilde{\mu}_{\mathrm{si}}, \tilde{\lambda}_{\mathrm{si}} &= \mu_{\mathrm{si}}/E_0, \lambda_{\mathrm{si}}/E_0 \\
\tilde{E}(c) = E_{\mathrm{si}}(1 + \eta_{\mathrm{E}}\chi_{\max}\tilde{c})/E_0, \text{ where } E_0 &= \frac{R_g T}{V_m^b} & & \\
\tilde{\sigma}_0 &= \frac{\sigma_0}{E_0} & & \\
\tilde{K} &= \frac{KH}{E_0} & & \\
\tilde{G}_0 &= \frac{G_0}{HE_0} & & \\
\tilde{\delta}_{\mathrm{initiation}} &= \frac{\delta_{\mathrm{initiation}}}{H} & & \\
\tilde{\delta}_{\mathrm{failure}} &= \frac{\delta_{\mathrm{failure}}}{H} & &
\end{aligned}$$

2.6 Definition of the state of charge

$$\begin{aligned}
\mathrm{soc} &= \frac{\int_{-L/2}^{L/2}\int_0^H \tilde{c}\mathrm{dydx}}{LH} && (61) \\
&= H^2 \frac{\int_{-L/2H}^{L/2H}\int_0^1 \tilde{c}(\tilde{x},\tilde{y})\mathrm{d\tilde{y}d\tilde{x}}}{LH} && (62) \\
&= H \frac{\int_{-L/2H}^{L/2H}\int_0^1 \tilde{c}(\tilde{x},\tilde{y})\mathrm{d\tilde{y}d\tilde{x}}}{L} && (63) \\
&= 2H \frac{\int_{0}^{L/2H}\int_0^1 \tilde{c}(\tilde{x},\tilde{y})\mathrm{d\tilde{y}d\tilde{x}}}{L} && (64) \\
&= \frac{2H}{L}\mathrm{intop1(\tilde{c})} && (65)
\end{aligned}$$

2.7 Equations in component form

$$\mathbf{F} = \begin{bmatrix} 1+\frac{\partial \tilde{u}}{\partial \tilde{X}} & \frac{\partial \tilde{u}}{\partial \tilde{Y}} & 0 \\ \frac{\partial \tilde{v}}{\partial \tilde{X}} & 1+\frac{\partial \tilde{v}}{\partial \tilde{Y}} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \tilde{F}_{11} & \tilde{F}_{12} & 0 \\ \tilde{F}_{21} & \tilde{F}_{22} & 0 \\ 0 & 0 & \tilde{F}_{33} \end{bmatrix} \tag{66}$$

$$\tilde{F}^{\mathrm{el}}_{11} = (J^c)^{-1/3}\lambda_{zz}(\tilde{F}_{11}\lambda_{yy} - \tilde{F}_{12}\lambda_{yx}) \tag{67}$$
$$\tilde{F}^{\mathrm{el}}_{12} = (J^c)^{-1/3}\lambda_{zz}(\tilde{F}_{12}\lambda_{xx} - \tilde{F}_{11}\lambda_{xy}) \tag{68}$$
$$\tilde{F}^{\mathrm{el}}_{21} = (J^c)^{-1/3}\lambda_{zz}(\tilde{F}_{21}\lambda_{yy} - \tilde{F}_{22}\lambda_{yx}) \tag{69}$$
$$\tilde{F}^{\mathrm{el}}_{22} = (J^c)^{-1/3}\lambda_{zz}(\tilde{F}_{22}\lambda_{xx} - \tilde{F}_{21}\lambda_{xy}) \tag{70}$$
$$\tilde{F}^{\mathrm{el}}_{33} = (J^c)^{-1/3}(1/\lambda_{zz})\tilde{F}_{33} \tag{71}$$

$$\tilde{E}^{\mathrm{el}}_{11} = 0.5[(\tilde{F}^{\mathrm{el}}_{11})^2 + (\tilde{F}^{\mathrm{el}}_{21})^2 - 1] \tag{72}$$
$$\tilde{E}^{\mathrm{el}}_{22} = 0.5[(\tilde{F}^{\mathrm{el}}_{12})^2 + (\tilde{F}^{\mathrm{el}}_{22})^2 - 1] \tag{73}$$
$$\tilde{E}^{\mathrm{el}}_{33} = 0.5[(\tilde{F}^{\mathrm{el}}_{33})^2 - 1] \tag{74}$$
$$\tilde{E}^{\mathrm{el}}_{12} = 0.5[\tilde{F}^{\mathrm{el}}_{11}\tilde{F}^{\mathrm{el}}_{12} + \tilde{F}^{\mathrm{el}}_{21}\tilde{F}^{\mathrm{el}}_{22}] = \tilde{E}^{\mathrm{el}}_{21} \tag{75}$$

$$\tilde{S}^{\mathrm{el}}_{11} = J^c[2\tilde{\mu}_{\mathrm{si}}(\tilde{c})\tilde{E}^{\mathrm{el}}_{11} + \tilde{\lambda}_{\mathrm{si}}(\tilde{c})(\tilde{E}^{\mathrm{el}}_{11} + \tilde{E}^{\mathrm{el}}_{22} + \tilde{E}^{\mathrm{el}}_{33})] \tag{76}$$
$$\tilde{S}^{\mathrm{el}}_{22} = J^c[2\tilde{\mu}_{\mathrm{si}}(\tilde{c})\tilde{E}^{\mathrm{el}}_{22} + \tilde{\lambda}_{\mathrm{si}}(\tilde{c})(\tilde{E}^{\mathrm{el}}_{11} + \tilde{E}^{\mathrm{el}}_{22} + \tilde{E}^{\mathrm{el}}_{33})] \tag{77}$$
$$\tilde{S}^{\mathrm{el}}_{33} = J^c[2\tilde{\mu}_{\mathrm{si}}(\tilde{c})\tilde{E}^{\mathrm{el}}_{33} + \tilde{\lambda}_{\mathrm{si}}(\tilde{c})(\tilde{E}^{\mathrm{el}}_{11} + \tilde{E}^{\mathrm{el}}_{22} + \tilde{E}^{\mathrm{el}}_{33})] \tag{78}$$
$$\tilde{S}^{\mathrm{el}}_{12} = J^c 2\tilde{\mu}_{\mathrm{si}}(\tilde{c})\tilde{E}^{\mathrm{el}}_{12} = \tilde{S}^{\mathrm{el}}_{21} \tag{79}$$
$$\tag{80}$$

$$\tilde{S}_{11} = (J^c)^{-2/3}[-\lambda_{xy}(\tilde{S}^{\mathrm{el}}_{12}\lambda_{yy} - \tilde{S}^{\mathrm{el}}_{22}\lambda_{xy}) + \lambda_{yy}(\tilde{S}^{\mathrm{el}}_{11}\lambda_{yy} - \tilde{S}^{\mathrm{el}}_{21}\lambda_{xy})]\lambda^2_{zz} \tag{81}$$
$$\tilde{S}_{12} = (J^c)^{-2/3}[\lambda_{xx}(\tilde{S}^{\mathrm{el}}_{12}\lambda_{yy} - \tilde{S}^{\mathrm{el}}_{22}\lambda_{xy}) - \lambda_{yx}(\tilde{S}^{\mathrm{el}}_{11}\lambda_{yy} - \tilde{S}^{\mathrm{el}}_{21}\lambda_{xy})]\lambda^2_{zz} \tag{82}$$
$$\tilde{S}_{21} = (J^c)^{-2/3}[\lambda_{xy}(\tilde{S}^{\mathrm{el}}_{12}\lambda_{yx} - \tilde{S}^{\mathrm{el}}_{22}\lambda_{xx}) - \lambda_{yy}(\tilde{S}^{\mathrm{el}}_{11}\lambda_{yx} - \tilde{S}^{\mathrm{el}}_{21}\lambda_{xx})]\lambda^2_{zz} \tag{83}$$
$$\tilde{S}_{22} = (J^c)^{-2/3}[-\lambda_{xx}(\tilde{S}^{\mathrm{el}}_{12}\lambda_{yx} - \tilde{S}^{\mathrm{el}}_{22}\lambda_{xx}) + \lambda_{yx}(\tilde{S}^{\mathrm{el}}_{11}\lambda_{yx} - \tilde{S}^{\mathrm{el}}_{21}\lambda_{xx})]\lambda^2_{zz} \tag{84}$$
$$\tilde{S}_{33} = (J^c)^{-2/3}\tilde{S}^{\mathrm{el}}_{33}/\lambda^2_{zz} \tag{85}$$

$$\tilde{P}_{11} = \tilde{F}_{11}\tilde{S}_{11} + \tilde{F}_{12}\tilde{S}_{21} \tag{86}$$
$$\tilde{P}_{12} = \tilde{F}_{11}\tilde{S}_{12} + \tilde{F}_{12}\tilde{S}_{22} \tag{87}$$
$$\tilde{P}_{21} = \tilde{F}_{21}\tilde{S}_{11} + \tilde{F}_{22}\tilde{S}_{21} \tag{88}$$
$$\tilde{P}_{22} = \tilde{F}_{21}\tilde{S}_{12} + \tilde{F}_{22}\tilde{S}_{22} \tag{89}$$
$$\tilde{P}_{33} = \tilde{F}_{33}\tilde{S}_{33} \tag{90}$$

$$
\begin{aligned}
J &= \tilde{F}_{33}(\tilde{F}_{11}\tilde{F}_{22} - \tilde{F}_{12}\tilde{F}_{21}) && (91)\\
\tilde{\sigma}_{11} &= (\tilde{F}_{11}\tilde{P}_{11} + \tilde{F}_{12}\tilde{P}_{12})/J && (92)\\
\tilde{\sigma}_{12} &= (\tilde{F}_{21}\tilde{P}_{11} + \tilde{F}_{22}\tilde{P}_{12})/J && (93)\\
\tilde{\sigma}_{21} &= (\tilde{F}_{11}\tilde{P}_{21} + \tilde{F}_{12}\tilde{P}_{22})/J && (94)\\
\tilde{\sigma}_{22} &= (\tilde{F}_{21}\tilde{P}_{21} + \tilde{F}_{22}\tilde{P}_{22})/J && (95)\\
\tilde{\sigma}_{33} &= \tilde{F}_{33}\tilde{P}_{33}/J && (96)\\
& && (97)
\end{aligned}
$$

$$
\begin{aligned}
\tilde{\tau}_{11} &= \tilde{\sigma}_{11} - (\tilde{\sigma}_{11} + \tilde{\sigma}_{22} + \tilde{\sigma}_{33})/3 && (98)\\
\tilde{\tau}_{22} &= \tilde{\sigma}_{22} - (\tilde{\sigma}_{11} + \tilde{\sigma}_{22} + \tilde{\sigma}_{33})/3 && (99)\\
\tilde{\tau}_{33} &= \tilde{\sigma}_{33} - (\tilde{\sigma}_{11} + \tilde{\sigma}_{22} + \tilde{\sigma}_{33})/3 && (100)\\
\tilde{\tau}_{12} &= \tilde{\tau}_{21} = \tilde{\sigma}_{12} && (101)
\end{aligned}
$$

$$
\tilde{\sigma}_{\mathrm{eff}} = \sqrt{\frac{3}{2}(\tilde{\tau}_{11}^2 + \tilde{\tau}_{22}^2 + \tilde{\tau}_{33}^2 + 2\tilde{\tau}_{12}^2)} \tag{102}
$$

$$
\begin{aligned}
\tilde{M}_{11}^{\mathrm{el}} &= J[-\tilde{F}_{12}^{\mathrm{el}}(\tilde{F}_{11}^{\mathrm{el}}\tilde{\tau}_{12} + \tilde{F}_{21}^{\mathrm{el}}\tilde{\tau}_{22}) + \tilde{F}_{22}^{\mathrm{el}}(\tilde{F}_{11}^{\mathrm{el}}\tilde{\tau}_{11} + \tilde{F}_{21}^{\mathrm{el}}\tilde{\tau}_{21})]/(\tilde{F}_{11}^{\mathrm{el}}\tilde{F}_{22}^{\mathrm{el}} - \tilde{F}_{12}^{\mathrm{el}}\tilde{F}_{21}^{\mathrm{el}}) && (103)\\
\tilde{M}_{12}^{\mathrm{el}} &= J[\tilde{F}_{11}^{\mathrm{el}}(\tilde{F}_{11}^{\mathrm{el}}\tilde{\tau}_{12} + \tilde{F}_{21}^{\mathrm{el}}\tilde{\tau}_{22}) - \tilde{F}_{21}^{\mathrm{el}}(\tilde{F}_{11}^{\mathrm{el}}\tilde{\tau}_{11} + \tilde{F}_{21}^{\mathrm{el}}\tilde{\tau}_{21})]/(\tilde{F}_{11}^{\mathrm{el}}\tilde{F}_{22}^{\mathrm{el}} - \tilde{F}_{12}^{\mathrm{el}}\tilde{F}_{21}^{\mathrm{el}}) && (104)\\
\tilde{M}_{21}^{\mathrm{el}} &= J[-\tilde{F}_{12}^{\mathrm{el}}(\tilde{F}_{12}^{\mathrm{el}}\tilde{\tau}_{12} + \tilde{F}_{22}^{\mathrm{el}}\tilde{\tau}_{22}) + \tilde{F}_{22}^{\mathrm{el}}(\tilde{F}_{12}^{\mathrm{el}}\tilde{\tau}_{11} + \tilde{F}_{22}^{\mathrm{el}}\tilde{\tau}_{21})]/(\tilde{F}_{11}^{\mathrm{el}}\tilde{F}_{22}^{\mathrm{el}} - \tilde{F}_{12}^{\mathrm{el}}\tilde{F}_{21}^{\mathrm{el}}) && (105)\\
\tilde{M}_{22}^{\mathrm{el}} &= J[\tilde{F}_{11}^{\mathrm{el}}(\tilde{F}_{12}^{\mathrm{el}}\tilde{\tau}_{12} + \tilde{F}_{22}^{\mathrm{el}}\tilde{\tau}_{22}) - \tilde{F}_{21}^{\mathrm{el}}(\tilde{F}_{12}^{\mathrm{el}}\tilde{\tau}_{11} + \tilde{F}_{22}^{\mathrm{el}}\tilde{\tau}_{21})]/(\tilde{F}_{11}^{\mathrm{el}}\tilde{F}_{22}^{\mathrm{el}} - \tilde{F}_{12}^{\mathrm{el}}\tilde{F}_{21}^{\mathrm{el}}) && (106)\\
\tilde{M}_{33}^{\mathrm{el}} &= J\tilde{\tau}_{33} && (107)
\end{aligned}
$$

Viscoplastic rates:

$$
\begin{aligned}
\dot{\lambda}_{xx} &= \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\mathrm{eff}}}(\tilde{M}_{11}^{\mathrm{el}}\lambda_{xx} + \tilde{M}_{12}^{\mathrm{el}}\lambda_{yx})\mathrm{H}(\frac{\tilde{\sigma}_{\mathrm{eff}}}{\tilde{\sigma}_{\mathrm{f}}} - 1)^{\mathrm{m}} && (108)\\
\dot{\lambda}_{xy} &= \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\mathrm{eff}}}(\tilde{M}_{11}^{\mathrm{el}}\lambda_{xy} + \tilde{M}_{12}^{\mathrm{el}}\lambda_{yy})\mathrm{H}(\frac{\tilde{\sigma}_{\mathrm{eff}}}{\tilde{\sigma}_{\mathrm{f}}} - 1)^{\mathrm{m}} && (109)\\
\dot{\lambda}_{yx} &= \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\mathrm{eff}}}(\tilde{M}_{21}^{\mathrm{el}}\lambda_{xx} + \tilde{M}_{22}^{\mathrm{el}}\lambda_{yx})\mathrm{H}(\frac{\tilde{\sigma}_{\mathrm{eff}}}{\tilde{\sigma}_{\mathrm{f}}} - 1)^{\mathrm{m}} && (110)\\
\dot{\lambda}_{yy} &= \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\mathrm{eff}}}(\tilde{M}_{21}^{\mathrm{el}}\lambda_{xy} + \tilde{M}_{22}^{\mathrm{el}}\lambda_{yy})\mathrm{H}(\frac{\tilde{\sigma}_{\mathrm{eff}}}{\tilde{\sigma}_{\mathrm{f}}} - 1)^{\mathrm{m}} && (111)\\
\dot{\lambda}_{zz} &= \frac{3\dot{d}_0\lambda_{zz}}{2J\tilde{\sigma}_{\mathrm{eff}}}\tilde{M}_{33}^{\mathrm{el}}\mathrm{H}(\frac{\tilde{\sigma}_{\mathrm{eff}}}{\tilde{\sigma}_{\mathrm{f}}} - 1)^{\mathrm{m}} && (112)\\
& && (113)
\end{aligned}
$$

Viscoplastic rate equations in non-dimensional form:

$$\frac{d\lambda_{xx}}{dt} = \frac{1}{t_{\mathrm{ref}}}\frac{d\lambda_{xx}}{d\tilde{t}} = \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\mathrm{eff}}}(\tilde{M}^{\mathrm{el}}_{11}\lambda_{xx} + \tilde{M}^{\mathrm{el}}_{12}\lambda_{yx})\mathrm{H}(\frac{\tilde{\sigma}_{\mathrm{eff}}}{\tilde{\sigma}_{\mathrm{f}}} - 1)^{\mathrm{m}} \tag{114}$$

$$\frac{d\lambda_{xx}}{d\tilde{t}} = \frac{3\dot{\tilde{d}}_0}{2J\tilde{\sigma}_{\mathrm{eff}}}(\tilde{M}^{\mathrm{el}}_{11}\lambda_{xx} + \tilde{M}^{\mathrm{el}}_{12}\lambda_{yx})\mathrm{H}(\frac{\tilde{\sigma}_{\mathrm{eff}}}{\tilde{\sigma}_{\mathrm{f}}} - 1)^{\mathrm{m}} \tag{115}$$

$$\text{where, } \dot{\tilde{d}}_0 = \dot{d}_0 t_{\mathrm{ref}} \tag{116}$$

Stress equilibrium Equation:

$$\boldsymbol{\nabla}_{\boldsymbol{X}} \cdot \mathbf{P} = \mathbf{0}. \tag{117}$$

$$\frac{\partial P_{11}}{\partial X} + \frac{\partial P_{12}}{\partial Y} = 0 \tag{118}$$

$$\text{and, } \frac{\partial P_{21}}{\partial X} + \frac{\partial P_{22}}{\partial Y} = 0 \tag{119}$$

In non-dimensional form:

$$\frac{E_0}{H}\frac{\partial \tilde{P}_{11}}{\partial \tilde{X}} + \frac{E_0}{H}\frac{\partial \tilde{P}_{12}}{\partial \tilde{Y}} = 0 \tag{120}$$

$$\text{and, } \frac{E_0}{H}\frac{\partial \tilde{P}_{21}}{\partial \tilde{X}} + \frac{E_0}{H}\frac{\partial \tilde{P}_{22}}{\partial \tilde{Y}} = 0 \tag{121}$$

So,

$$\frac{\partial \tilde{P}_{11}}{\partial \tilde{X}} + \frac{\partial \tilde{P}_{12}}{\partial \tilde{Y}} = 0 \tag{122}$$

$$\text{and, } \frac{\partial \tilde{P}_{21}}{\partial \tilde{X}} + \frac{\partial \tilde{P}_{22}}{\partial \tilde{Y}} = 0 \tag{123}$$

Mass conservation Equation:

$$\frac{\partial c}{\partial t} = -\boldsymbol{\nabla}_{\boldsymbol{X}} \cdot \boldsymbol{j} = -(\frac{\partial j_x}{\partial X} + \frac{\partial j_y}{\partial Y}) \tag{124}$$

For one way coupling:

$$\boldsymbol{j} = -D_0 \boldsymbol{\nabla}_{\boldsymbol{X}} c \tag{125}$$

$$\tilde{j}_x = j_x H/(c_{\mathrm{max}} D_0) \tag{126}$$

$$= -D_0 \frac{\partial c}{\partial X} H/(c_{\mathrm{max}} D_0) \tag{127}$$

$$= -\frac{\partial \tilde{c}}{\partial \tilde{X}} \tag{128}$$

$$\tilde{j}_y = j_y H/(c_{\mathrm{max}} D_0) \tag{129}$$

$$= -\frac{\partial \tilde{c}}{\partial \tilde{Y}} \tag{130}$$

For two way coupling:

$$\boldsymbol{j} = -\frac{1}{R_g T}\frac{D\chi_{\max}\tilde{c}}{V_m^b}(F)^{-1}(F)^{-\mathsf{T}}\boldsymbol{\nabla}_{\boldsymbol{X}}\mu \tag{131}$$

$$D = D_0\exp(\frac{\alpha \mathrm{S_h}}{\mathrm{E_0}}) \tag{132}$$

$$\mu = \mu_0 + \mu_s \tag{133}$$

$$\mu_0 = R_g T\log(\gamma\tilde{c}) \tag{134}$$

$$\gamma = \frac{1}{1-\tilde{c}}\exp(\frac{1}{R_g T}[2(A_0 - 2B_0)\tilde{c} - 3(A_0 - B_0)(\tilde{c}^2)]) \tag{135}$$

$$\mu_s = \frac{V_m^b}{\chi_{\max}}[-\frac{1}{3}\frac{\partial J^c}{\partial\tilde{c}}\tilde{F}^{\mathrm{el}}_{im}\tilde{F}^{\mathrm{el}}_{in}C_{mnkl}\tilde{E}^{\mathrm{el}}_{kl} + \frac{1}{2}(J^c\frac{\partial C_{ijkl}}{\partial\tilde{c}} + \frac{\partial J^c}{\partial\tilde{c}}C_{ijkl})\tilde{E}^{\mathrm{el}}_{ij}\tilde{E}^{\mathrm{el}}_{kl}] \tag{136}$$

$$= (\mu_1 + \mu_2 + \mu_3)/\chi_{\max} \tag{137}$$

$$\tilde{\mu} = \tilde{\mu}_0 + (\tilde{\mu}_1 + \tilde{\mu}_2 + \tilde{\mu}_3)/\chi_{\max} \tag{138}$$

$$\tilde{\mu}_0 = \log(\gamma\tilde{c}) \tag{139}$$

$$\tilde{\mu}_1 = -\frac{1}{6(J^c)}\frac{\partial J^c}{\partial\tilde{c}}[\tilde{S}^{\mathrm{el}}_{11}\tilde{E}^{\mathrm{el}}_{11} + \tilde{S}^{\mathrm{el}}_{22}\tilde{E}^{\mathrm{el}}_{22} + 2\tilde{S}^{\mathrm{el}}_{12}\tilde{E}^{\mathrm{el}}_{12} + \tilde{S}^{\mathrm{el}}_{33}\tilde{E}^{\mathrm{el}}_{33}] \tag{140}$$

$$\tilde{\mu}_2 = -\frac{1}{3(J^c)}\frac{\partial J^c}{\partial\tilde{c}}[\tilde{S}^{\mathrm{el}}_{11} + \tilde{S}^{\mathrm{el}}_{22} + \tilde{S}^{\mathrm{el}}_{33}] \tag{141}$$

$$\tilde{\mu}_3 = \frac{1}{2}J^c\frac{\partial\tilde{C}_{ijkl}}{\partial\tilde{c}}\tilde{E}^{\mathrm{el}}_{kl}\tilde{E}^{\mathrm{el}}_{ij} \tag{142}$$

$$= \frac{1}{2}J^c[2\tilde{\mu}'_{\mathrm{si}}(\tilde{c})\tilde{E}^{\mathrm{el}}_{ij}\tilde{E}^{\mathrm{el}}_{ij} + \tilde{\lambda}'_{\mathrm{si}}(\tilde{c})(\tilde{E}^{\mathrm{el}}_{11} + \tilde{E}^{\mathrm{el}}_{22} + \tilde{E}^{\mathrm{el}}_{33})\tilde{E}^{\mathrm{el}}_{ij}\delta_{ij}] \tag{143}$$

$$= \frac{1}{2}J^c[2\tilde{\mu}'_{\mathrm{si}}(\tilde{c})((\tilde{E}^{\mathrm{el}}_{11})^2 + (\tilde{E}^{\mathrm{el}}_{22})^2 + (\tilde{E}^{\mathrm{el}}_{33})^2 + 2(\tilde{E}^{\mathrm{el}}_{12})^2) + \tilde{\lambda}'_{\mathrm{si}}(c)(\tilde{E}^{\mathrm{el}}_{11} + \tilde{E}^{\mathrm{el}}_{22} + \tilde{E}^{\mathrm{el}}_{33})^2] \tag{144}$$

$$\boldsymbol{j} = -\frac{D\chi_{\max}\tilde{c}}{V_m^b}\tilde{\mathbf{F}}^{-1}(\tilde{\mathbf{F}}^{-1})^{\mathsf{T}}\nabla_{\boldsymbol{X}}\tilde{\mu} \tag{145}$$

$$\tilde{\boldsymbol{j}} = \boldsymbol{j}HV_m^b/(\chi_{\max}D_0) \tag{146}$$

$$= -\frac{D}{D_0}H\tilde{c}\tilde{\mathbf{F}}^{-1}(\tilde{\mathbf{F}}^{-1})^{\mathsf{T}}\nabla_{\boldsymbol{X}}\tilde{\mu} \tag{147}$$

$$\tilde{j}_x = \frac{-\bar{D}H\tilde{c}}{J^2}\left(\frac{\partial\tilde{\mu}}{\partial X}(\tilde{F}^2_{12} + \tilde{F}^2_{22}) - \frac{\partial\tilde{\mu}}{\partial Y}(\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22})\right) \tag{148}$$

$$= \frac{-\bar{D}\tilde{c}}{J^2}\left(\frac{\partial\tilde{\mu}}{\partial\tilde{X}}(\tilde{F}^2_{12} + \tilde{F}^2_{22}) - \frac{\partial\tilde{\mu}}{\partial\tilde{Y}}(\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22})\right) \tag{149}$$

$$\tilde{j}_y = \frac{-\bar{D}H\tilde{c}}{J^2}\left(\frac{\partial\tilde{\mu}}{\partial Y}(\tilde{F}^2_{11} + \tilde{F}^2_{21}) - \frac{\partial\tilde{\mu}}{\partial X}(\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22})\right) \tag{150}$$

$$= \frac{-\bar{D}\tilde{c}}{J^2}\left(\frac{\partial\tilde{\mu}}{\partial\tilde{Y}}(\tilde{F}^2_{11} + \tilde{F}^2_{21}) - \frac{\partial\tilde{\mu}}{\partial\tilde{X}}(\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22})\right) \tag{151}$$

$$\tag{152}$$

In non-dimensional form:

$$c_{\max}\frac{D_0}{H^2}\frac{\partial\tilde{c}}{\partial\tilde{t}} = -(\frac{1}{H}\frac{\partial\tilde{j}_x}{\partial\tilde{X}} + \frac{1}{H}\frac{\partial\tilde{j}_y}{\partial\tilde{Y}})c_{\max}\frac{D_0}{H} \tag{153}$$

$$\text{so, } \frac{\partial\tilde{c}}{\partial\tilde{t}} = -(\frac{\partial\tilde{j}_x}{\partial\tilde{X}} + \frac{\partial\tilde{j}_y}{\partial\tilde{Y}}) \tag{154}$$

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

$$\tilde{\mathbf{F}}_X = \frac{\partial\tilde{\mathbf{F}}}{\partial\tilde{X}} = \begin{bmatrix} \frac{\partial^2\tilde{u}}{\partial\tilde{X}^2} & \frac{\partial^2\tilde{u}}{\partial\tilde{X}\tilde{Y}} & 0 \\ \frac{\partial^2\tilde{v}}{\partial\tilde{X}^2} & \frac{\partial^2\tilde{v}}{\partial\tilde{X}\tilde{Y}} & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{155}$$

$$\tilde{\mathbf{F}}_Y = \frac{\partial\tilde{\mathbf{F}}}{\partial\tilde{Y}} = \begin{bmatrix} \frac{\partial^2\tilde{u}}{\partial\tilde{X}\tilde{Y}} & \frac{\partial^2\tilde{u}}{\partial\tilde{Y}^2} & 0 \\ \frac{\partial^2\tilde{v}}{\partial\tilde{X}\tilde{Y}} & \frac{\partial^2\tilde{v}}{\partial\tilde{Y}^2} & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{156}$$

$$\tilde{F}^{\mathrm{el}}_{11_x} = -\frac{1}{3}(J^c)^{-4/3}\frac{dJ^c}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}F_{11} + (J^c)^{-1/3}F_{11_x} \tag{157}$$

$$\tilde{F}^{\mathrm{el}}_{12_x} = -\frac{1}{3}(J^c)^{-4/3}\frac{dJ^c}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}F_{12} + (J^c)^{-1/3}F_{12_x} \tag{158}$$

$$\tilde{F}^{\mathrm{el}}_{21_x} = -\frac{1}{3}(J^c)^{-4/3}\frac{dJ^c}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}F_{21} + (J^c)^{-1/3}F_{21_x} \tag{159}$$

$$\tilde{F}^{\mathrm{el}}_{22_x} = -\frac{1}{3}(J^c)^{-4/3}\frac{dJ^c}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}F_{22} + (J^c)^{-1/3}F_{22_x} \tag{160}$$

$$\tilde{F}^{\mathrm{el}}_{33_x} = \tag{161}$$

$$\tilde{E}^{\mathrm{el}}_{11_x} = \tilde{F}^{\mathrm{el}}_{11}\tilde{F}^{\mathrm{el}}_{11_x} + \tilde{F}^{\mathrm{el}}_{21}\tilde{F}^{\mathrm{el}}_{21_x} \tag{162}$$

$$\tilde{E}^{\mathrm{el}}_{22_x} = \tilde{F}^{\mathrm{el}}_{12}\tilde{F}^{\mathrm{el}}_{12_x} + \tilde{F}^{\mathrm{el}}_{22}\tilde{F}^{\mathrm{el}}_{22_x} \tag{163}$$

$$\tilde{E}^{\mathrm{el}}_{12_x} = 0.5[\tilde{F}^{\mathrm{el}}_{11_x}\tilde{F}^{\mathrm{el}}_{12} + \tilde{F}^{\mathrm{el}}_{11}\tilde{F}^{\mathrm{el}}_{12_x} + \tilde{F}^{\mathrm{el}}_{21_x}\tilde{F}^{\mathrm{el}}_{22} + \tilde{F}^{\mathrm{el}}_{21}\tilde{F}^{\mathrm{el}}_{22_x}] = \tilde{E}^{\mathrm{el}}_{21_x} \tag{164}$$

$$\tilde{E}^{\mathrm{el}}_{33_x} = \tag{165}$$

$$\tilde{E}^{\mathrm{el}}_{trace} = \tilde{E}^{\mathrm{el}}_{11} + \tilde{E}^{\mathrm{el}}_{22} + \tilde{E}^{\mathrm{el}}_{33} \tag{166}$$

$$\tilde{E}^{\mathrm{el}}_{trace_x} = \tilde{E}^{\mathrm{el}}_{11_x} + \tilde{E}^{\mathrm{el}}_{22_x} + \tilde{E}^{\mathrm{el}}_{33_x} \tag{167}$$

$$\tilde{S}^{\text{el}}_{11_x} = \frac{dJ^c}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\frac{\tilde{S}^{\text{el}}_{11}}{J^c} + J^c\left(2\frac{d\tilde{\mu}_{si}}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\tilde{E}^{\text{el}}_{11} + 2\tilde{\mu}_{si}\tilde{E}^{\text{el}}_{11_x} + \frac{d\tilde{\lambda}_{si}}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\tilde{E}^{\text{el}}_{trace} + \tilde{\lambda}_{si}\tilde{E}^{\text{el}}_{trace_x}\right) \tag{168}$$

$$\tilde{S}^{\text{el}}_{22_x} = \frac{dJ^c}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\frac{\tilde{S}^{\text{el}}_{22}}{J^c} + J^c\left(2\frac{d\tilde{\mu}_{si}}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\tilde{E}^{\text{el}}_{22} + 2\tilde{\mu}_{si}\tilde{E}^{\text{el}}_{22_x} + \frac{d\tilde{\lambda}_{si}}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\tilde{E}^{\text{el}}_{trace} + \tilde{\lambda}_{si}\tilde{E}^{\text{el}}_{trace_x}\right) \tag{169}$$

$$\tilde{S}^{\text{el}}_{33_x} = \frac{dJ^c}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\frac{\tilde{S}^{\text{el}}_{33}}{J^c} + J^c\left(2\frac{d\tilde{\mu}_{si}}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\tilde{E}^{\text{el}}_{33} + 2\tilde{\mu}_{si}\tilde{E}^{\text{el}}_{33_x} + \frac{d\tilde{\lambda}_{si}}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\tilde{E}^{\text{el}}_{trace} + \tilde{\lambda}_{si}\tilde{E}^{\text{el}}_{trace_x}\right) \tag{170}$$

$$\tilde{S}^{\text{el}}_{12_x} = 2\frac{dJ^c}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\tilde{\mu}_{si}\tilde{E}^{\text{el}}_{12} + 2J^c\frac{d\tilde{\mu}_{si}}{d\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\tilde{E}^{\text{el}}_{12} + 2J^c\tilde{\mu}_{si}\tilde{E}^{\text{el}}_{12_x} = \tilde{S}^{\text{el}}_{21_x} \tag{171}$$

$$\gamma = \frac{1}{1-\tilde{c}}\exp(\frac{1}{R_gT}[2(A_0-2B_0)\tilde{c} - 3(A_0-B_0)(\tilde{c}^2)]) \tag{172}$$

$$\frac{\partial\gamma}{\partial\tilde{X}} = \gamma_x = \frac{1}{(1-\tilde{c})^2}\frac{\partial\tilde{c}}{\partial\tilde{X}}\exp(...) + \frac{1}{1-\tilde{c}}\exp(...)\frac{1}{R_gT}[2(A_0-2B_0)\frac{\partial\tilde{c}}{\partial\tilde{X}} - 3(A_0-B_0)(2\tilde{c}\frac{\partial\tilde{c}}{\partial\tilde{X}})] \tag{173}$$

$$= \frac{1}{1-\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}}\gamma + \frac{\gamma}{R_gT}[2(A_0-2B_0)\frac{\partial\tilde{c}}{\partial\tilde{X}} - 3(A_0-B_0)(2\tilde{c}\frac{\partial\tilde{c}}{\partial\tilde{X}})] \tag{174}$$

$$\tag{175}$$

$$\tilde{\mu}_0 = \log(\gamma\tilde{c}) \tag{176}$$

$$\tilde{\mu}_{0_x} = \frac{1}{\gamma}\gamma_x + \frac{1}{\tilde{c}}\frac{\partial\tilde{c}}{\partial\tilde{X}} \tag{177}$$

$$\tilde{\mu}_1 = -\frac{1}{6(J^c)}\frac{\partial J^c}{\partial\tilde{c}}[\tilde{S}^{\text{el}}_{11}\tilde{E}^{\text{el}}_{11} + \tilde{S}^{\text{el}}_{22}\tilde{E}^{\text{el}}_{22} + 2\tilde{S}^{\text{el}}_{12}\tilde{E}^{\text{el}}_{12} + \tilde{S}^{\text{el}}_{33}\tilde{E}^{\text{el}}_{33}] \tag{178}$$

$$= -\frac{1}{2J^c}\eta\chi_{\max}[\tilde{S}^{\text{el}}_{11}\tilde{E}^{\text{el}}_{11} + \tilde{S}^{\text{el}}_{22}\tilde{E}^{\text{el}}_{22} + 2\tilde{S}^{\text{el}}_{12}\tilde{E}^{\text{el}}_{12} + \tilde{S}^{\text{el}}_{33}\tilde{E}^{\text{el}}_{33}] \tag{179}$$

$$\tilde{\mu}_{1_x} = (-\frac{1}{2}\eta\chi_{\max}) * (-\frac{1}{{J^c}^2}3\eta\chi_{\max}) * \frac{\partial\tilde{c}}{\partial\tilde{X}}[...] - \frac{1}{2J^c}\eta\chi_{\max}[...]_x \tag{180}$$

$$= -3\eta\chi_{\max}\frac{1}{J^c}\frac{\partial\tilde{c}}{\partial\tilde{X}}\tilde{\mu}_1 - \eta\chi_{\max}\frac{1}{2J^c}[\tilde{S}^{\text{el}}_{11_x}\tilde{E}^{\text{el}}_{11} + \tilde{S}^{\text{el}}_{11}\tilde{E}^{\text{el}}_{11_x} + \tilde{S}^{\text{el}}_{22_x}\tilde{E}^{\text{el}}_{22} + \tilde{S}^{\text{el}}_{22}\tilde{E}^{\text{el}}_{22_x} \tag{181}$$

$$+\tilde{S}^{\text{el}}_{33_x}\tilde{E}^{\text{el}}_{33} + \tilde{S}^{\text{el}}_{33}\tilde{E}^{\text{el}}_{33_x} + 2\tilde{S}^{\text{el}}_{12_x}\tilde{E}^{\text{el}}_{12} + 2\tilde{S}^{\text{el}}_{12}\tilde{E}^{\text{el}}_{12_x}] \tag{182}$$

$$\tilde{\mu}_2 = -\frac{1}{3(J^c)}\frac{\partial J^c}{\partial\tilde{c}}[\tilde{S}^{\text{el}}_{11} + \tilde{S}^{\text{el}}_{22} + \tilde{S}^{\text{el}}_{33}] \tag{183}$$

$$= -\frac{1}{J^c}\eta\chi_{\max}[\tilde{S}^{\text{el}}_{11} + \tilde{S}^{\text{el}}_{22} + \tilde{S}^{\text{el}}_{33}] \tag{184}$$

$$\tilde{\mu}_{2_x} = -\frac{3\eta\chi_{\max}}{J^c}\frac{\partial\tilde{c}}{\partial\tilde{X}}\tilde{\mu}_2 - \frac{\eta\chi_{\max}}{J^c}[\tilde{S}^{\text{el}}_{11_x} + \tilde{S}^{\text{el}}_{22_x} + \tilde{S}^{\text{el}}_{33_x}] \tag{185}$$

$$\tilde{\mu}_3 = \frac{1}{2} J^c [2\tilde{\mu}'_{\mathrm{si}}(\tilde{c})((\tilde{E}^{\mathrm{el}}_{11})^2 + (\tilde{E}^{\mathrm{el}}_{22})^2 + (\tilde{E}^{\mathrm{el}}_{33})^2 + 2(\tilde{E}^{\mathrm{el}}_{12})^2) + \tilde{\lambda}'_{\mathrm{si}}(c)(\tilde{E}^{\mathrm{el}}_{11} + \tilde{E}^{\mathrm{el}}_{22} + \tilde{E}^{\mathrm{el}}_{33})^2] \tag{186}$$

$$\tilde{\mu}_{3_x} = \frac{dJ^c}{d\tilde{c}} \frac{\partial \tilde{c}}{\partial \tilde{X}} \frac{\tilde{\mu}_3}{J^c} + \frac{J^c}{2} \left[2\tilde{\mu}'_{\mathrm{si}}(2\tilde{E}^{\mathrm{el}}_{11}\tilde{E}^{\mathrm{el}}_{11_x} + 2\tilde{E}^{\mathrm{el}}_{22}\tilde{E}^{\mathrm{el}}_{22_x} + 2\tilde{E}^{\mathrm{el}}_{33}\tilde{E}^{\mathrm{el}}_{33_x} + 4\tilde{E}^{\mathrm{el}}_{12}\tilde{E}^{\mathrm{el}}_{12_x}) + 2\tilde{\lambda}'_{\mathrm{si}}(\tilde{E}^{\mathrm{el}}_{trace}\tilde{E}^{\mathrm{el}}_{trace_x})) \right] \tag{187}$$

$$\tilde{\mu}_x = \tilde{\mu}_{0_x} + (\tilde{\mu}_{1_x} + \tilde{\mu}_{2_x} + \tilde{\mu}_{3_x})/\chi_{\mathrm{max}} \tag{188}$$

2.8 Boundary and Initial Conditions

$$\tilde{c}(\tilde{X}, \tilde{Y}, 0) = 0 \tag{189}$$

$$\tilde{u}(\tilde{X}, \tilde{Y}, 0) = 0 \tag{190}$$

$$\tilde{v}(\tilde{X}, \tilde{Y}, 0) = 0 \tag{191}$$

$$\tilde{u}(\tilde{X}, 0, \tilde{t}) = \tilde{v}(\tilde{X}, 0, \tilde{t}) = 0; \text{ all three other faces are traction free} \tag{192}$$

$$\tilde{j}_x(\tilde{X}, 1, \tilde{t}) = \tilde{j}_0(1 - \tilde{c}(\tilde{X}, 1, \tilde{t})); \text{ all three other faces are insulated from any flux} \tag{193}$$