Extended calculations

For simplicity

$$R = c - u - v, c = c_\infty$$

I'll show that

$$\mu_u = \ln u - \ln R$$

I will skip the constants in free energy

$$F = u\ln\frac{u}{R} + v\ln\frac{v}{R} + c\ln\left(1 - \frac{u+v}{c}\right) = u\ln u - u\ln R + v\ln v - v\ln R + c\ln R - c\ln c$$

So

$$F = u\ln u - u\ln R + v\ln v - v\ln R + c\ln R - c\ln c$$

$$\mu_u = \frac{\partial F}{\partial u}$$

The derivatives are

We add them all together and get

$$\begin{aligned}
&\frac{\partial}{\partial u}(u\ln u) = \ln u + 1,\\
&\frac{\partial}{\partial u}(-u\ln R) = -\ln R + \frac{u}{R},\ \text{(the mistakes were here)}\\
&\frac{\partial}{\partial u}(v\ln v) = 0,\\
&\frac{\partial}{\partial u}(-v\ln R) = \frac{v}{R},\\
&\frac{\partial}{\partial u}(c\ln R) = -\frac{c}{R},\\
&\frac{\partial}{\partial u}(-c\ln c) = 0.
\end{aligned}$$

$$\ln u + 1 - \ln R + \frac{u+v-c}{R} = \ln u - \ln R + 1 - \frac{R}{R} = \ln u - \ln R$$

$$\mu_u = \ln u - \ln R = \ln u - \ln(c - u - v)$$

Now we compute derivative

We have

$$\partial_x\mu_u = \frac{u'}{u} - \frac{R'}{R} = \left(\frac{1}{u} + \frac{1}{R}\right)u' + \frac{1}{R}v'$$

Then

$$u\partial_x\mu_u = u' - \frac{uR'}{R} = (1+\frac{u}{R})u' + \frac{u}{R}v' = u' + \frac{u}{R}(u'+v')$$

So we would get

$$\begin{aligned} D_{uu} &= (1+\frac{u}{R}) = 1 + \frac{u}{c-u-v} \\ D_{uv} &= \frac{u}{R} = \frac{u}{c-u-v} \end{aligned}$$

We would have to

So

$$\begin{aligned} \partial_x(u\partial_x\mu_u) &= u'' + \frac{u'R - R'u}{R^2}(u'+v') + \frac{u}{R}(u''+v'') \\ &= u'' + \frac{u'}{R}(u'+v') + \frac{u}{R^2}(u'+v')^2 + \frac{u}{R}(u''+v'') \\ &= u'' - \frac{u(RR''-(R')^2) + R'u'R}{R^2} \\ &= u'' - \frac{u}{R}R'' + u\frac{(R')^2}{R^2} - \frac{R'u'}{R} \end{aligned}$$

Or finally

$$\partial_x(u\partial_x\mu_u) = u'' + \frac{u'}{(c-u-v)}(u'+v') + \frac{u}{(c-u-v)^2}(u'+v')^2 + \frac{u}{(c-u-v)}(u''+v'')$$

And from this we get the linearization $u \to u + \delta u$, by also assuming $u', v', u'', v'' = 0$ and ignoring higher order terms.

$$\delta\dot{u} = \delta u'' + \frac{u}{c-u-v}(\delta u'' + \delta v'') + \text{ reaction kinetics part}$$

If we introduce the coefficient in free energy we'll get

$$\delta\dot{u} = D\left(\delta u'' + \frac{u}{c-u-v}(\delta u'' + \delta v'')\right) + \text{ reaction kinetics part}$$

Or

$$\delta\dot{u} = D_{uu}\delta u'' + D_{uv}\delta v'' + \dots$$

ie. for $\delta w = (\delta u, \delta v)$

$$\delta \dot{w} = D \begin{pmatrix} 1 + \frac{u}{c-v-v} & \frac{u}{c-v-v} \\ \frac{v}{c-u-v} & 1 + \frac{v}{c-u-v} \end{pmatrix} \delta w'' + \text{ reaction kinetics part}$$

So the end result is the same