Compute derivatives for 1/S k - terms.

Express the individual k – tems in 1/S in terms of D_k, T_k & P_k

In[25]:=
```
OoSi[Dk_, Tk_, Pk_, U0_] = (J / (Ea M)) Dk (Ea / J)^Pk (Tk U0^Tk Log[U0] - U0^Tk + 1) / Tk^2
```

Out[25]=
$$\frac{Dk \left(\frac{Ea}{J}\right)^{Pk} J \left(1 - U0^{Tk} + Tk\, U0^{Tk} \text{Log}[U0]\right)}{Ea\, M\, Tk^2}$$

In[30]:=
```
Simplify[OoSi[Dk, Tk, Pk, U0] == (J / (Ea M)) Dk (Ea / J)^Pk (U0^Tk (Tk Log[U0] - 1) + 1) / Tk^2]
```

Out[30]= True

Now express the individual terms in terms of functions of J, M and U_0

In[27]:=
```
OoSi[Dk[J], Tk[J, m], Pk[J], U0]
```

Out[27]=
$$\frac{\left(\frac{Ea}{J}\right)^{Pk[J]} J\, Dk[J] \left(1 - U0^{Tk[J,m]} + U0^{Tk[J,m]} \text{Log}[U0]\, Tk[J, m]\right)}{Ea\, M\, Tk[J, m]^2}$$

Take the derivative wrt to m.

In[31]:=
```
D[OoSi[Dk[J], Tk[J, m], Pk[J], U0], m]
```

Out[31]=
$$\frac{\left(\frac{Ea}{J}\right)^{Pk[J]} J\, U0^{Tk[J,m]}\, Dk[J]\, \text{Log}[U0]^2\, Tk^{(0,1)}[J, m]}{Ea\, M\, Tk[J, m]} - \frac{2 \left(\frac{Ea}{J}\right)^{Pk[J]} J\, Dk[J] \left(1 - U0^{Tk[J,m]} + U0^{Tk[J,m]} \text{Log}[U0]\, Tk[J, m]\right) Tk^{(0,1)}[J, m]}{Ea\, M\, Tk[J, m]^3}$$

In[32]:=
```
2 (Ea / J)^Pk[J] J Dk[J] (1 - U0^Tk[J,m] + U0^Tk[J,m] Log[U0] Tk[J, m]) Tk^(0,1)[J, m] / (Ea M Tk[J, m]^3) /
 OoSi[Dk[J], Tk[J, m], Pk[J], U0]
```

Out[32]=
$$\frac{2\, Tk^{(0,1)}[J, m]}{Tk[J, m]}$$

Re - factor the derivative to make it easier to calculate

In[34]:=
```
Simplify[D[OoSi[Dk[J], Tk[J, m], Pk[J], U0], m] ==
 ((J / (Ea M)) U0^Tk[J,m] (Ea / J)^Pk[J] Dk[J] Log[U0]^2 - 2 OoSi[Dk[J], Tk[J, m], Pk[J], U0])
  (Tk^(0,1)[J, m] / Tk[J, m])]
```

Out[34]= True

Take the derivative wrt to J.

In[35]:=
```
D[OoSi[Dk[J], Tk[J, m], Pk[J], U0], J]
```

Out[35]=
$$\frac{\left(\frac{Ea}{J}\right)^{Pk[J]}\,Dk[J]\,\left(1-U0^{Tk[J,m]}+U0^{Tk[J,m]}\,Log[U0]\,Tk[J,m]\right)}{Ea\,M\,Tk[J,m]^2}+$$
$$\frac{\left(\frac{Ea}{J}\right)^{Pk[J]}\,J\,\left(1-U0^{Tk[J,m]}+U0^{Tk[J,m]}\,Log[U0]\,Tk[J,m]\right)\,Dk'[J]}{Ea\,M\,Tk[J,m]^2}+$$
$$\frac{\left(\frac{Ea}{J}\right)^{Pk[J]}\,J\,Dk[J]\,\left(1-U0^{Tk[J,m]}+U0^{Tk[J,m]}\,Log[U0]\,Tk[J,m]\right)\,\left(-\frac{Pk[J]}{J}+Log\left[\frac{Ea}{J}\right]\,Pk'[J]\right)}{Ea\,M\,Tk[J,m]^2}+$$
$$\frac{\left(\frac{Ea}{J}\right)^{Pk[J]}\,J\,U0^{Tk[J,m]}\,Dk[J]\,Log[U0]^2\,Tk^{(1,0)}[J,m]}{Ea\,M\,Tk[J,m]}-$$
$$\frac{2\,\left(\frac{Ea}{J}\right)^{Pk[J]}\,J\,Dk[J]\,\left(1-U0^{Tk[J,m]}+U0^{Tk[J,m]}\,Log[U0]\,Tk[J,m]\right)\,Tk^{(1,0)}[J,m]}{Ea\,M\,Tk[J,m]^3}$$

In[36]:=
```
(Ea/J)^Pk[J] Dk[J] (1 - U0^Tk[J,m] + U0^Tk[J,m] Log[U0] Tk[J, m]) / (Ea M Tk[J, m]^2) / OoSi[Dk[J], Tk[J, m], Pk[J], U0]
```

Out[36]=
$$\frac{1}{J}$$

In[37]:=
```
(Ea/J)^Pk[J] J (1 - U0^Tk[J,m] + U0^Tk[J,m] Log[U0] Tk[J, m]) Dk'[J] / (Ea M Tk[J, m]^2) / OoSi[Dk[J], Tk[J, m], Pk[J], U0]
```

Out[37]=
$$\frac{Dk'[J]}{Dk[J]}$$

In[38]:=
```
(Ea/J)^Pk[J] J Dk[J] (1 - U0^Tk[J,m] + U0^Tk[J,m] Log[U0] Tk[J, m]) (-Pk[J]/J + Log[Ea/J] Pk'[J]) / (Ea M Tk[J, m]^2) /
 OoSi[Dk[J], Tk[J, m], Pk[J], U0]
```

Out[38]=
$$-\frac{Pk[J]}{J}+Log\left[\frac{Ea}{J}\right]\,Pk'[J]$$

In[39]:=
```
2 (Ea/J)^Pk[J] J Dk[J] (1 - U0^Tk[J,m] + U0^Tk[J,m] Log[U0] Tk[J, m]) Tk^(1,0)[J, m] / (Ea M Tk[J, m]^3) /
 OoSi[Dk[J], Tk[J, m], Pk[J], U0]
```

Out[39]=
$$\frac{2\,Tk^{(1,0)}[J,m]}{Tk[J,m]}$$

Re - factor the derivative to make it easier to calculate

In[41]:=
```
Simplify[D[OoSi[Dk[J], Tk[J, m], Pk[J], U0], J] ==
  (((1/J + Dk'[J]/Dk[J] + Log[Ea/J]) Pk'[J] - Pk[J]/J - 2 Tk^(1,0)[J, m]/Tk[J, m]) OoSi[Dk[J], Tk[J, m], Pk[J], U0] +
    ((J/(Ea M)) U0^Tk[J,m] (Ea/J)^Pk[J] Dk[J] Log[U0]^2 Tk^(1,0)[J, m])/Tk[J, m])]
```

Out[41]= True

Take the derivative wrt to U_0. (Remember the U_0 in the multiplier in front of the sum...)

In[42]:=
```
D[OoSi[Dk[J], Tk[J, m], Pk[J], U0], U0]
```

Out[42]=
$$\frac{\left(\frac{Ea}{J}\right)^{Pk[J]}\ J\ U0^{-1+Tk[J,m]}\ Dk[J]\ Log[U0]}{Ea\ M}$$

In[44]:=
```
Simplify[
  D[OoSi[Dk[J], Tk[J, m], Pk[J], U0], U0] == (((J/(Ea M)) U0^Tk[J,m] (Ea/J)^Pk[J] Dk[J] Log[U0])/U0)]
```

Out[44]= True