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DISEQUILIBRIUM AS HABITABILITY SIGN: AN INTEGRATED TOOL

Talk outline:

[>> *EXTENT OF LOCAL DISEQUILIBRIUM* <<]

* LSs mineralogical description
* Gibbs free energy analysis
* Entropy production analysis
* Future work during MSL operations
* Favorite LS

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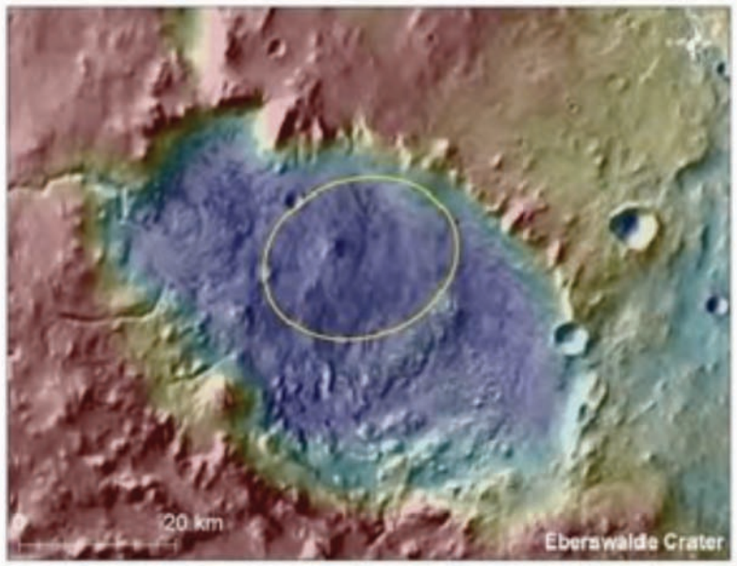
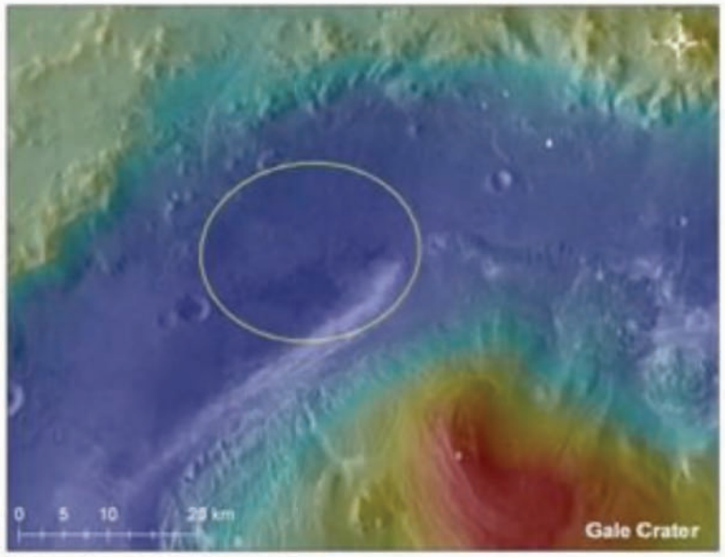
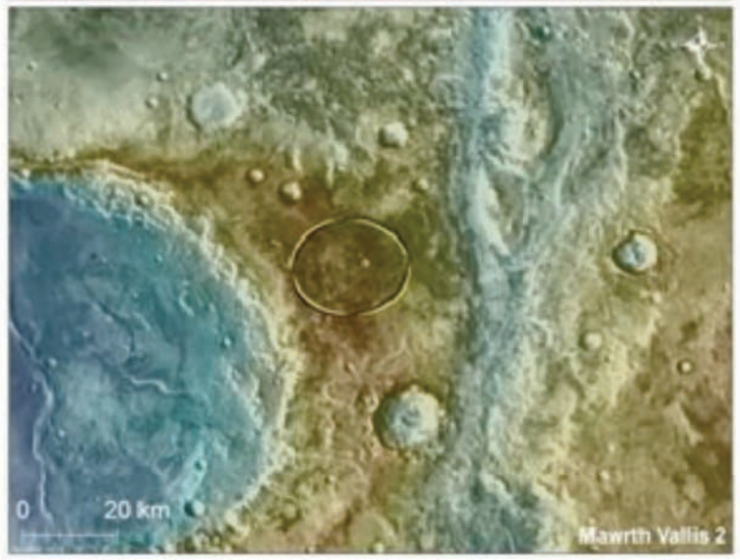
Landing Sites Mineralogy

Eberswalde Crater
=> *Olivine, Sulfate*

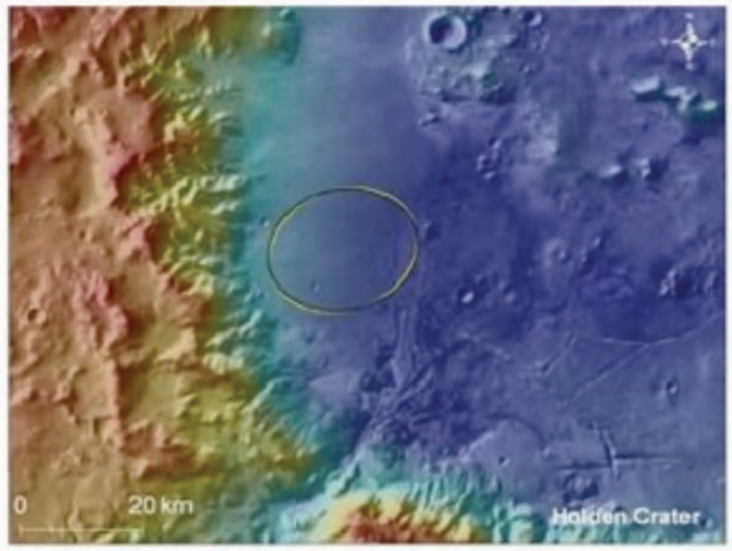


Gale Crater
=> *Olivine, Sulfate*





Mawrth Vallis
=> *Hematite*



Holden Crater
=> *Olivine, Sulfate*

Olivine => Fe(II)
Sulfate => SO_4^{2-}
Hematite => Fe(III)

$H_2S + 2\ O_2 \leftrightharpoons SO_4^{2-} + 2\ H^+$	R1
$FeS_2 + H_2O + 3.5\ O_2 \leftrightharpoons Fe^{2+} + 2\ SO_4^{2-} + 2H^+$	R2
$SO_4^{2-} + 2\ H^+ + 4\ H_2 \leftrightharpoons H_2S + 4\ H_2O$	R3
$Fe^{2+} + 0.25\ O_2 + H^+ \leftrightharpoons Fe^{3+} + 0.5\ H_2O$	R4
$Fe^{2+} + H_2O + 0.25\ O_2 \leftrightharpoons 0.5\ \text{Hematite} + 2\ H^+$	R5
$Fe^{3+} + 0.5\ H_2 \leftrightharpoons Fe^{2+} + H^+$	R6
$\text{Goethite} + 2\ H^+ + 0.5\ H_2 \leftrightharpoons 2\ H_2O + Fe^{2+}$	R7
$H_2 + 0.5\ O_2 \leftrightharpoons H_2O$	R8
$CH_4 + 2\ O_2 \leftrightharpoons 2\ H_2O + CO_2$	R9
$CO_2 + 4\ H_2 \leftrightharpoons 2\ H_2O + CH_4$	R10

A.D. Rogers, J.L. Bandfield, Icarus 203 (2009)

Methods - Gibbs Free Energy

Chemical Potential:
Temperature + Pressure Dependence

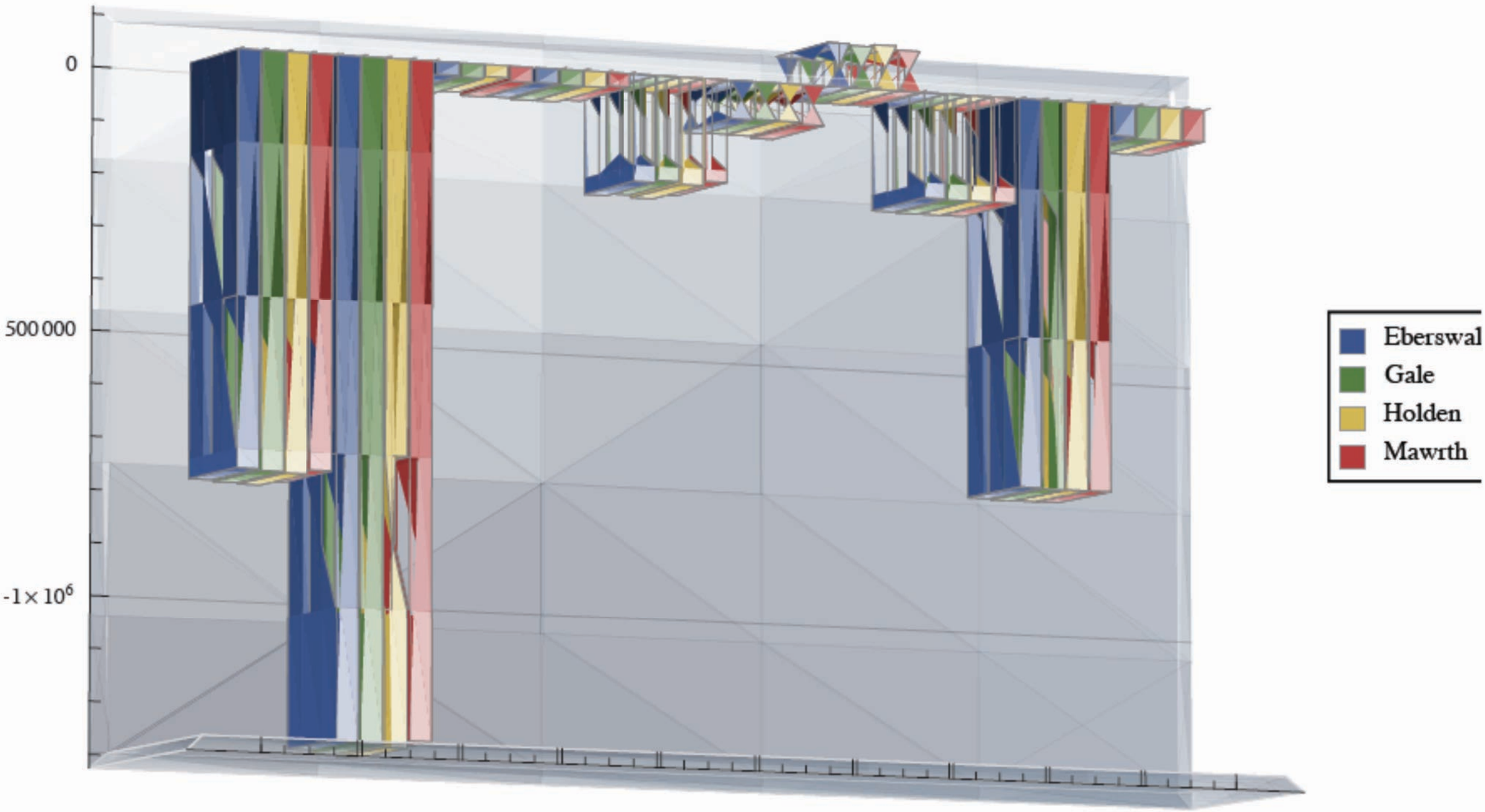
$$\mu_{0,k}(p,T) = RT\ln(\tfrac{p}{p_0}) + \tfrac{T}{T_0}(\mu_{0,k}(p_0,T_0) - \Delta H_k(p_0,T_0)) + \Delta H_k(p_0,T_0)$$

Local Conditions:

Landing Site	1	2	3	4	5	6	7
Eberswalde	0.25	0.92	0.75	0.67	0.67	0.00	0.00
Gale	0.00	0.83	1.00	0.83	0.83	0.00	0.00
Holden	0.17	1.17	0.83	1.00	1.00	0.00	0.00
	0.25	1.25	0.75	1.00	1.00	0.00	0.00
Mawrth	0.00	0.50	1.00	0.50	0.50	0.43	0.43
	0.00	0.00	1.00	0.00	0.00	1.00	1.00

Kondepudi, D., Prigogine, I.: Modern Thermodynamics. Wiley, NY, 1998.

Results - Gibbs Free Energy



Methods - Extent of Chemical Disequilibrium

$$\mathrm{A} + \mathrm{B} \; {}^{k_f}\!\rightleftharpoons_{k_r} \; \mathrm{C} + \mathrm{D}$$

$$Rf = k_f[A][B] \quad Rr = k_r[C][D]$$

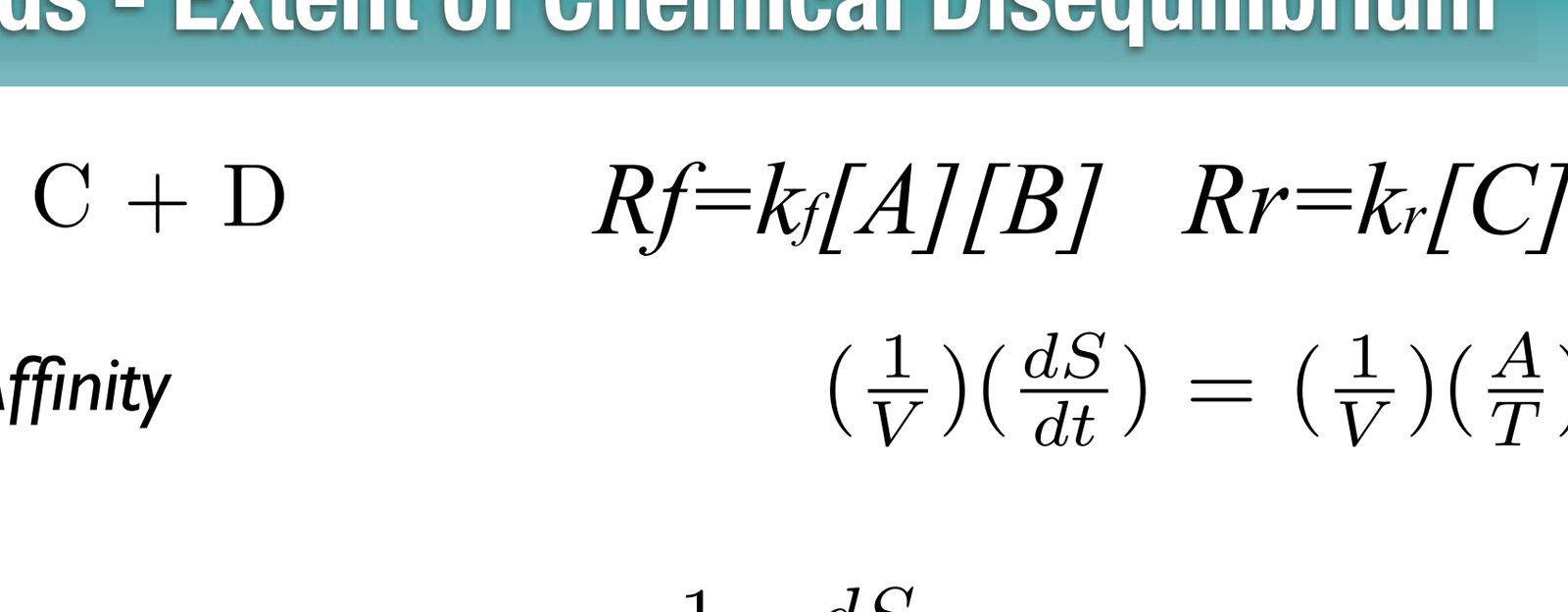
A = Chemical Affinity

$$\left(\frac{1}{V}\right)\left(\frac{dS}{dt}\right) = \left(\frac{1}{V}\right)\left(\frac{A}{T}\right)\left(\frac{d\zeta}{dt}\right)$$

$$k_r = \frac{k_f}{e^{-\frac{\Delta G^0}{RT}}}$$

$$\left(\frac{1}{V}\right)\left(\frac{dS}{dt}\right) = R(Rf - Rr)ln\left(\frac{Rf}{Rr}\right)$$

$$\frac{dS}{dt}\Big|_{t_{equilibrium}}$$

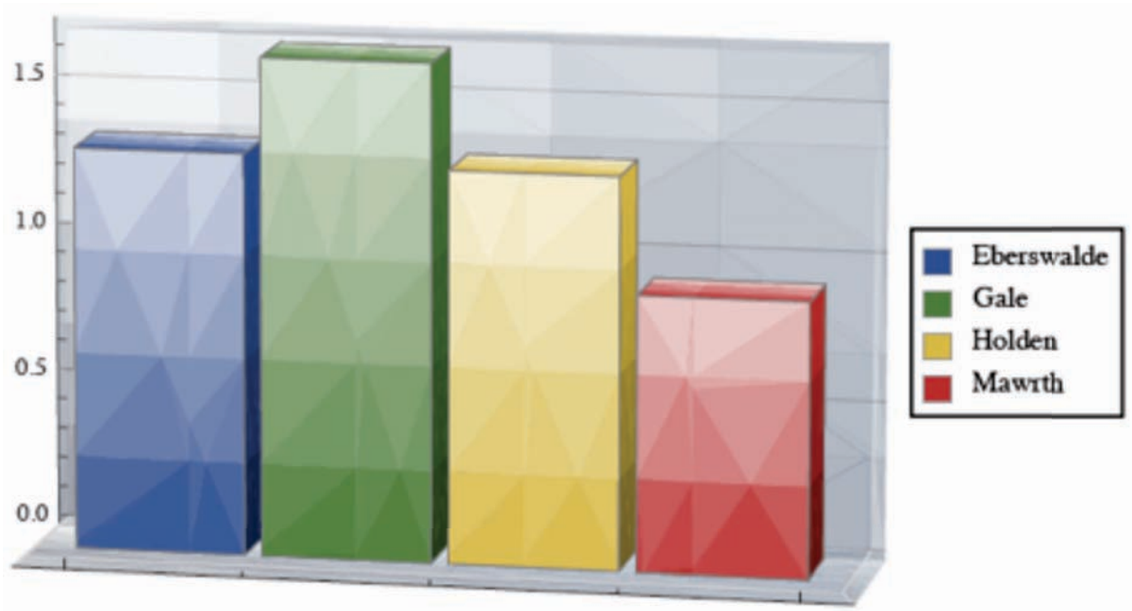


Kondepudi, D., Prigogine, I.: Modern Thermodynamics. Wiley, NY, 1998.

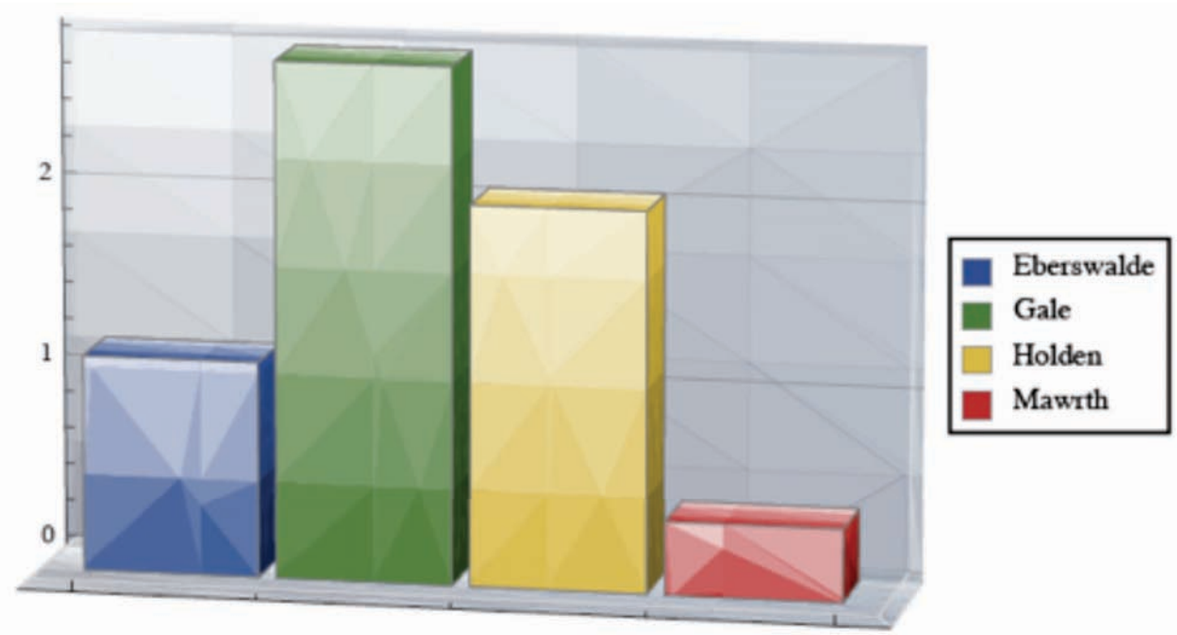
Results - Extent of Chemical Disequilibrium

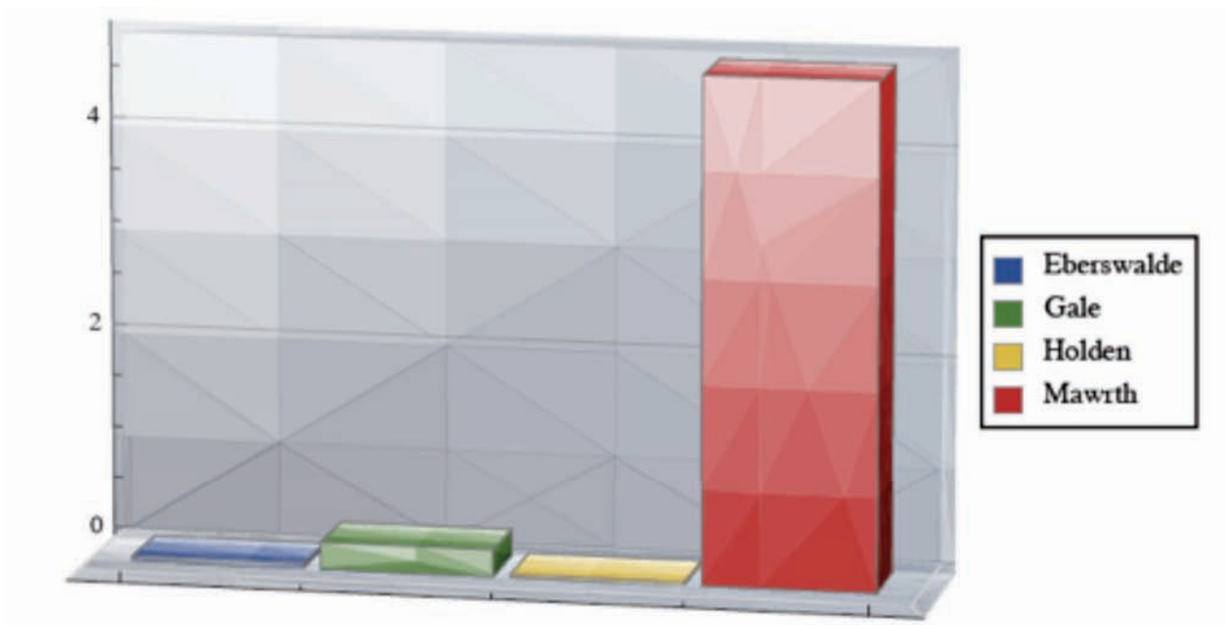
$$\Delta S(JK^{-1}L^{-1})$$

B1 (*10^{-61})

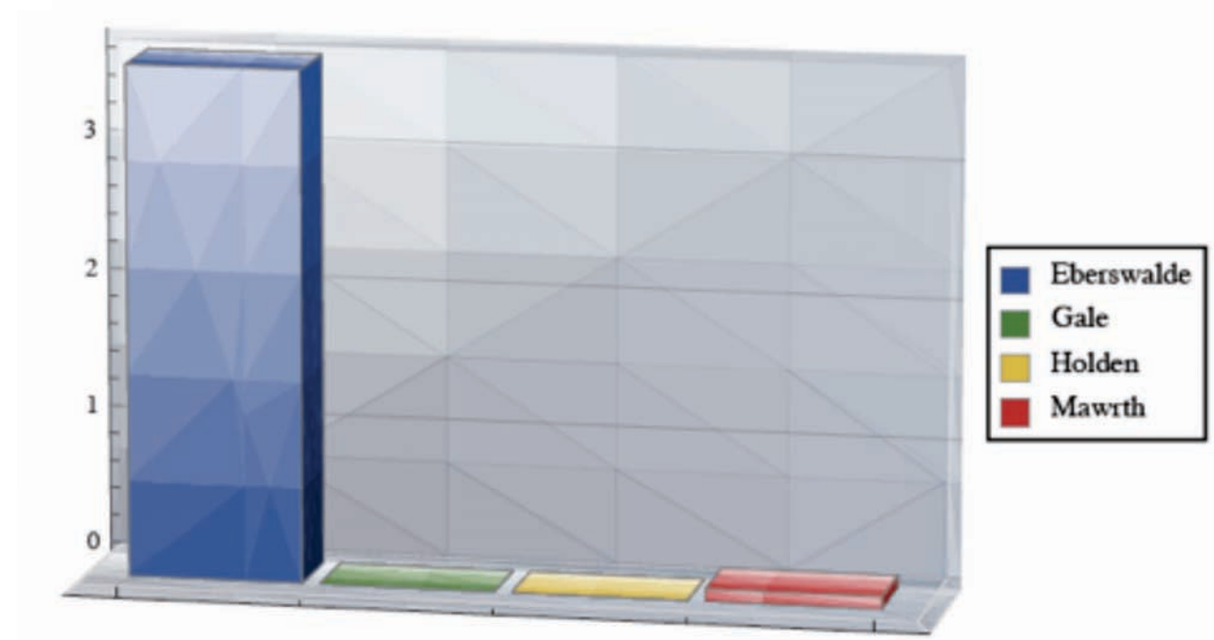


B2 (*10^{-58})





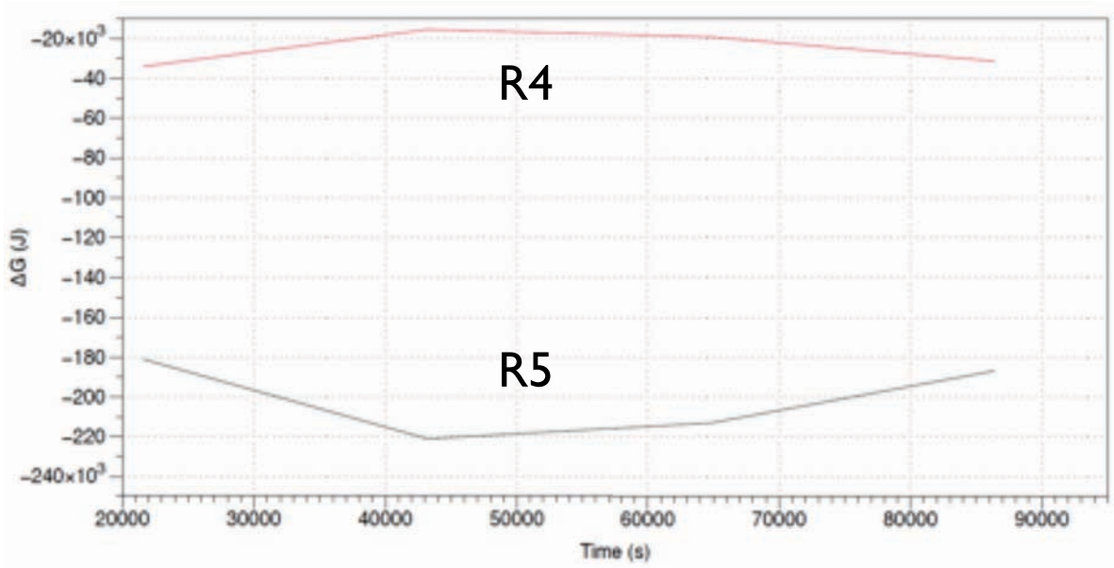
B4 (*10^{-6})



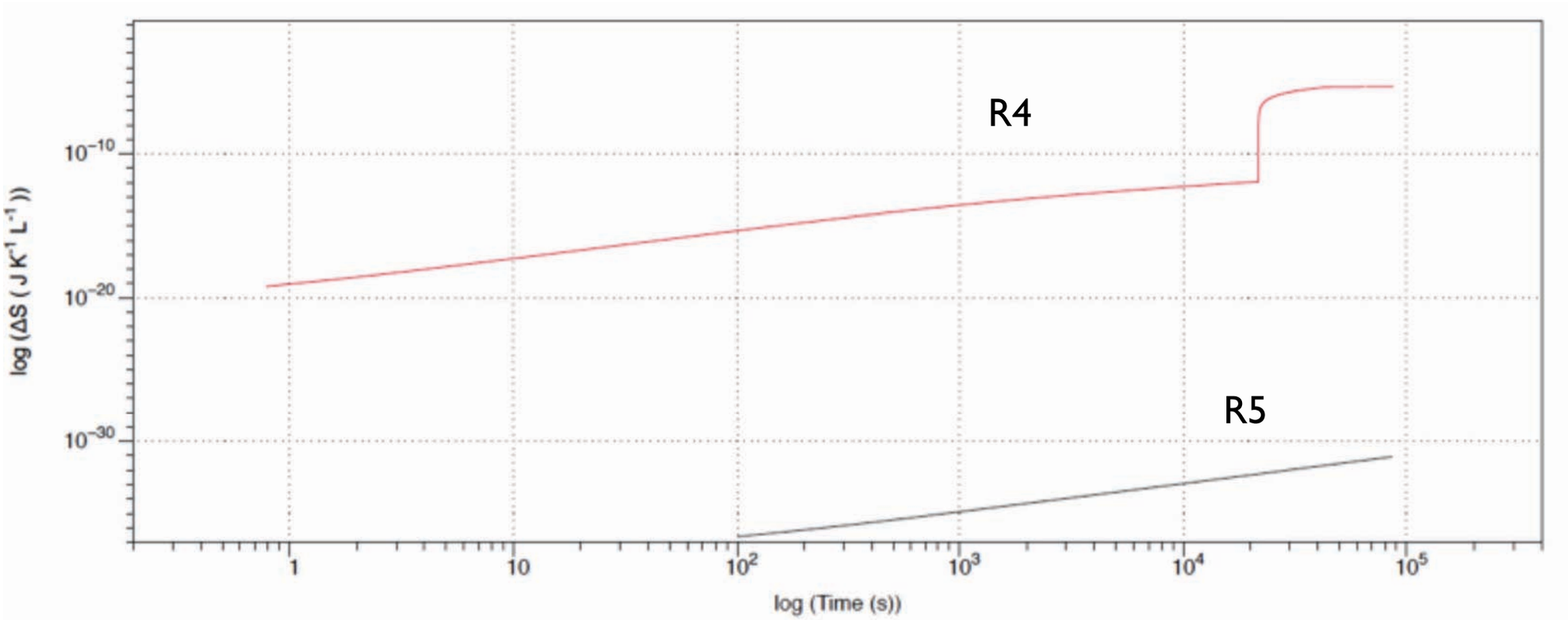
B5 (*10^{-30})

Improving: dG and dS as complementary methods

dG variation during a Martian Day



Entropy production during a Martian Day
(log/log comparison)



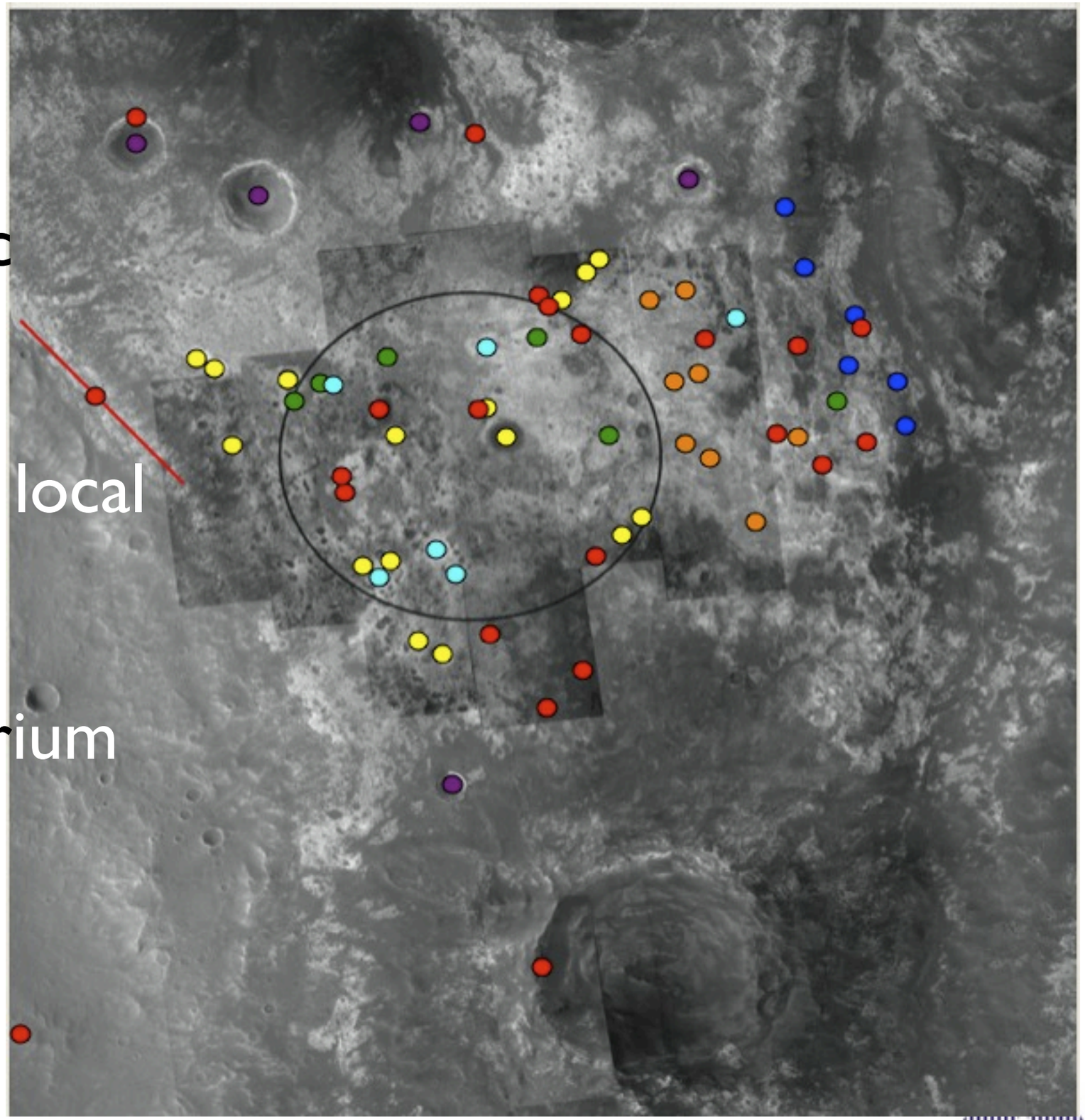
Future work

Mawrth Vallis targets

=> Targets' specific conditions

=> Characterization of local disequilibrium

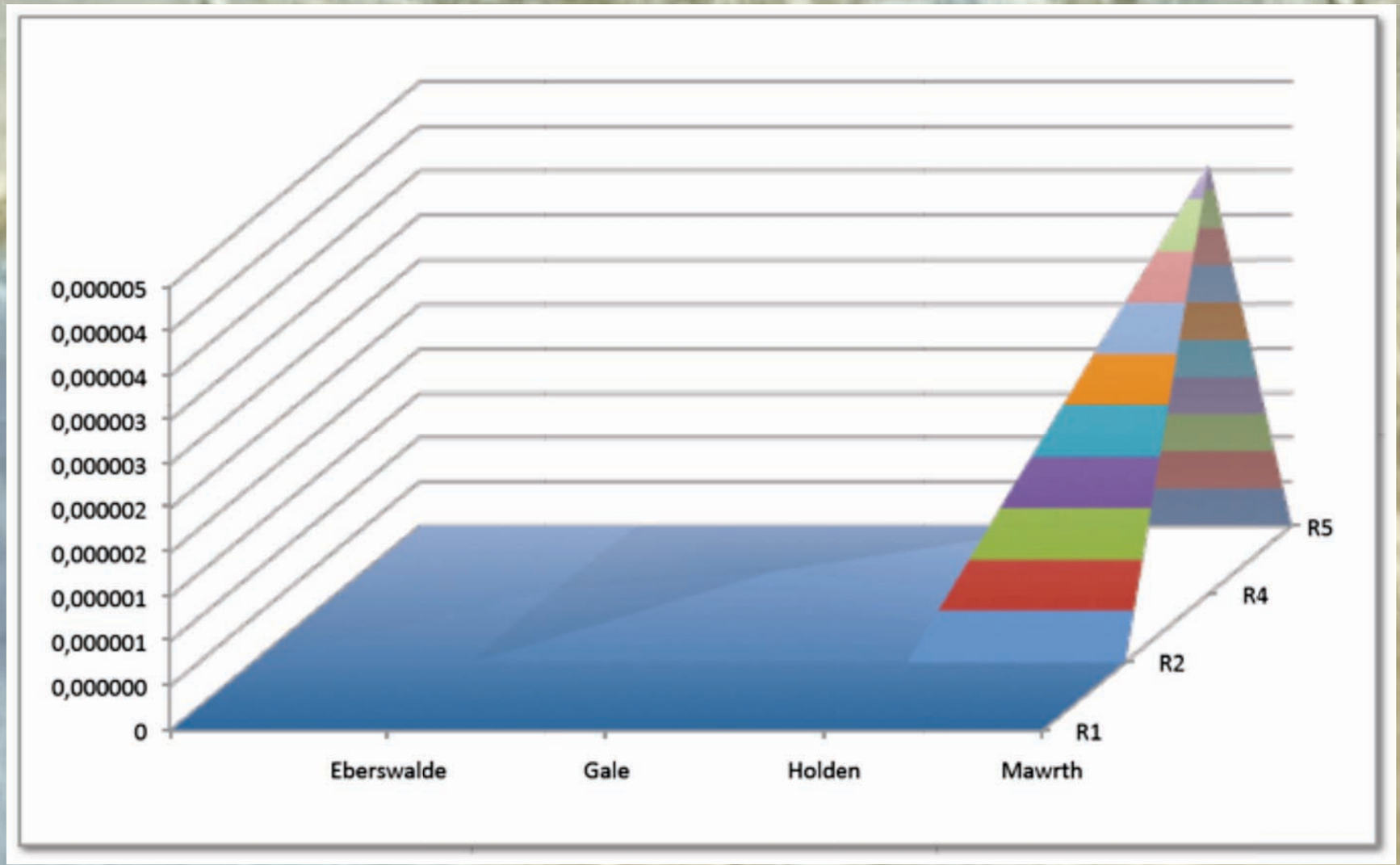
=> Draw a "disequilibrium map"



Landing Site with Largest Entropy Production

Mawrth Vallis

higher disequilibrium available (mostly by Fe(II) oxidation)



THANKS !