Structural Geology & Resources 2022
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Mineral systems as chemical reactors with no mathematics

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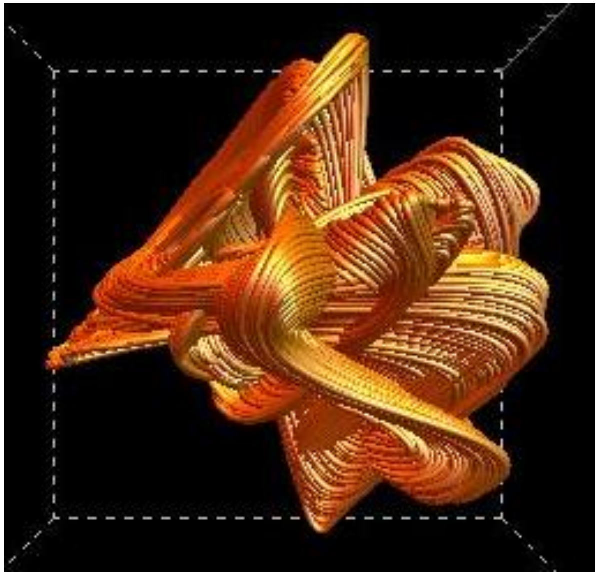
Session 4. 10.45 – 12.30

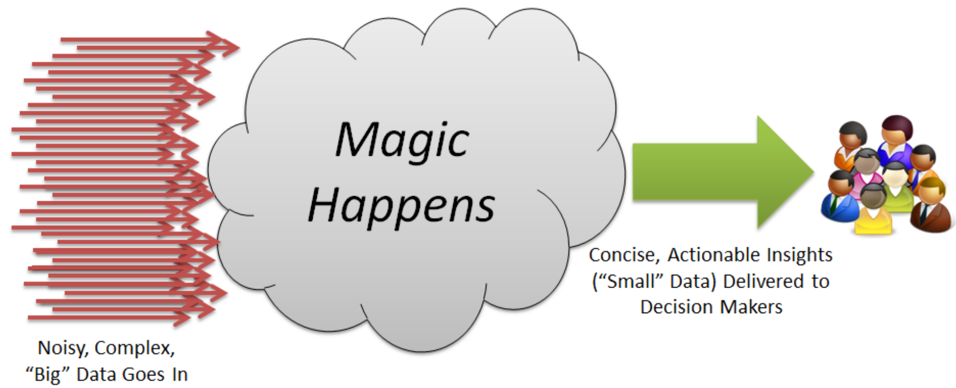
The nonlinear toolbox: What do we do with all these data?

- Wavelets and multifractals. Long range correlations.
- Recurrence.
- **Probability distributions**

Fingerprint for a mineralising system



Probability distributions.



"This red line indicates the change in this red line over a period of time."

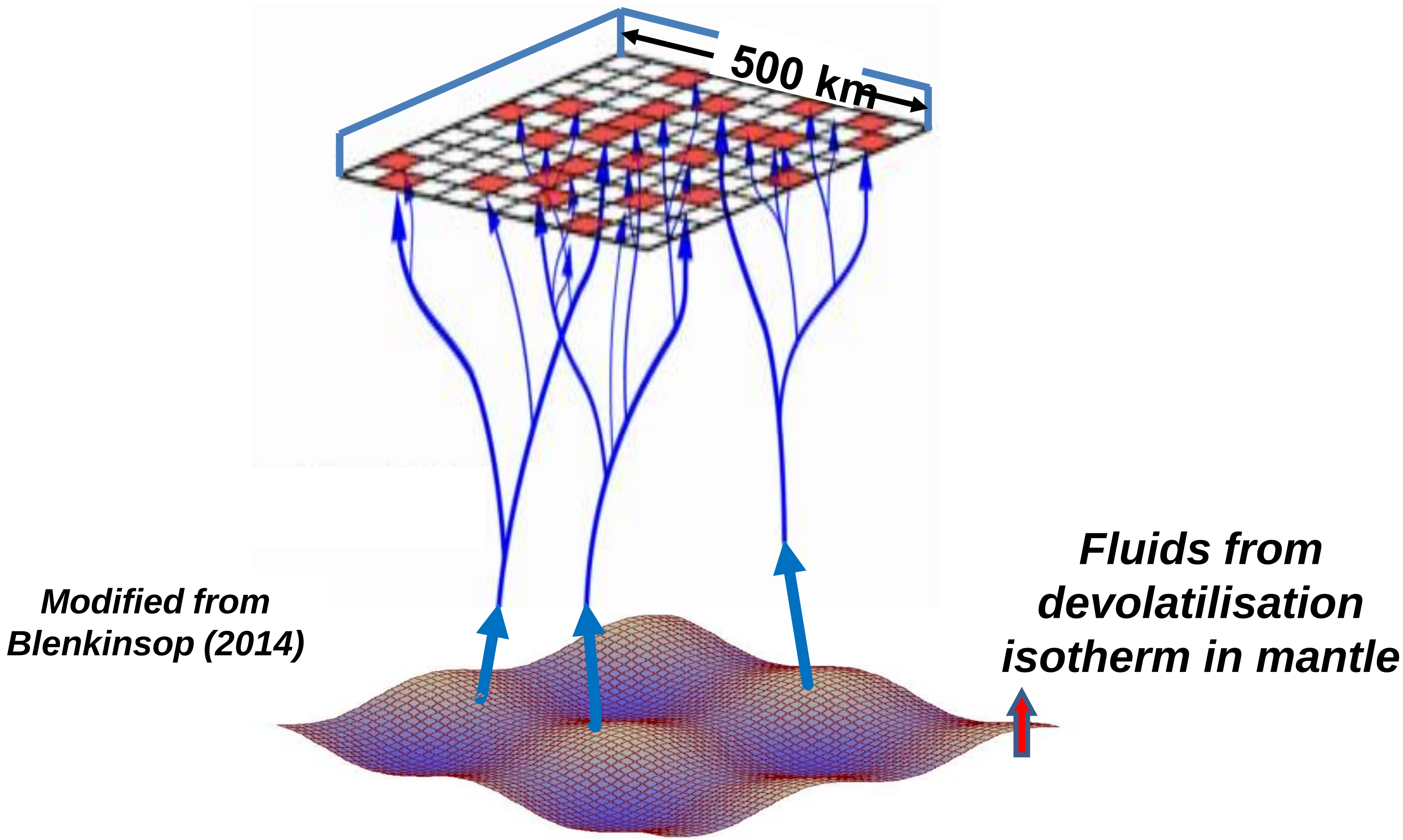
This is Mr Smith from Big Data Mining.
He says he's found an insight.

Probability distributions are the third important tool that have a direct link to the processes that operated in a mineralising system.

The interactions in mineralising systems are nonlinear (each has an influence on others) and hence the probability distributions that develop are a reflection of these interactions. As Savageau (1979, 1980) showed:

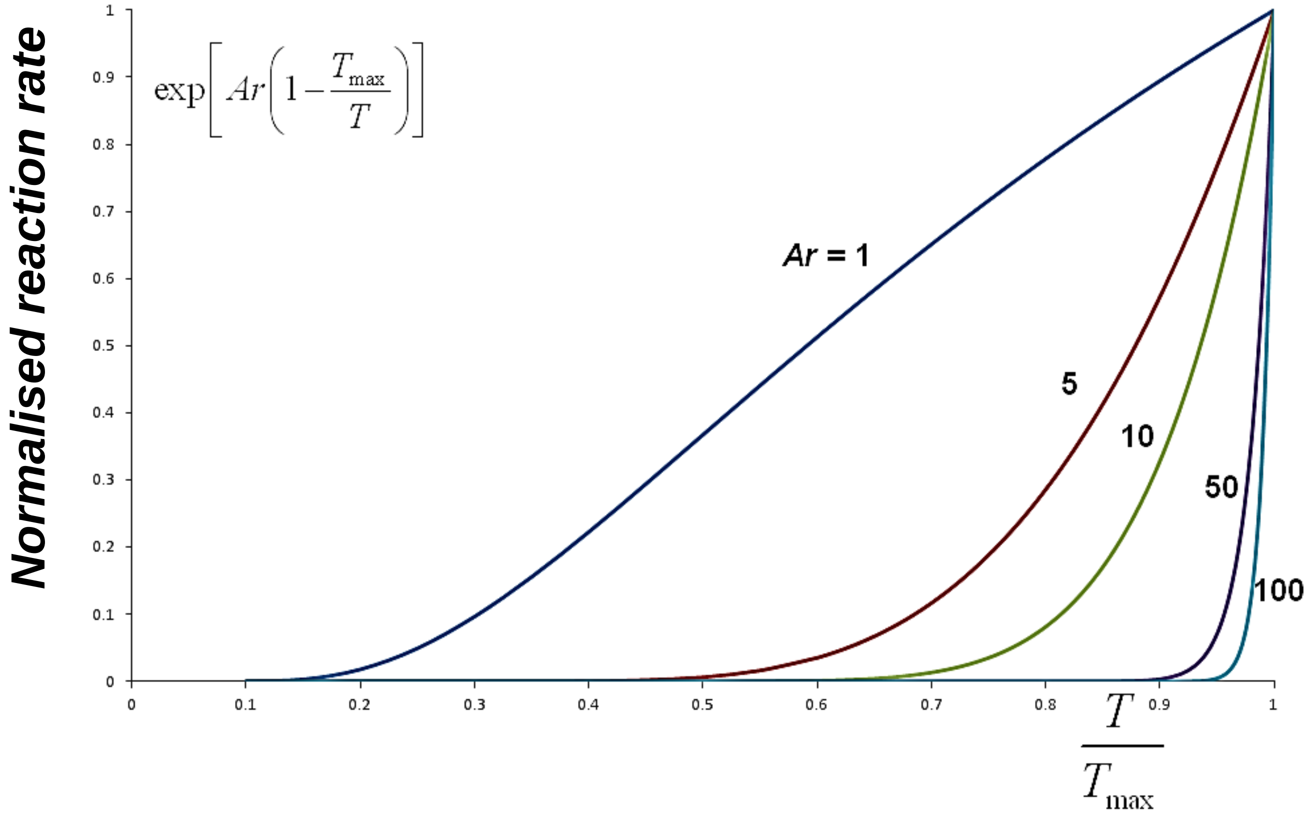
Any nonlinear system that grows to maturity has a growth curve that is a legitimate cumulative probability distribution.

What are the growth laws associated with mineralising systems?



Nucleation → Growth controlled by supply of heat/mass → Extinction

Reaction kinetics



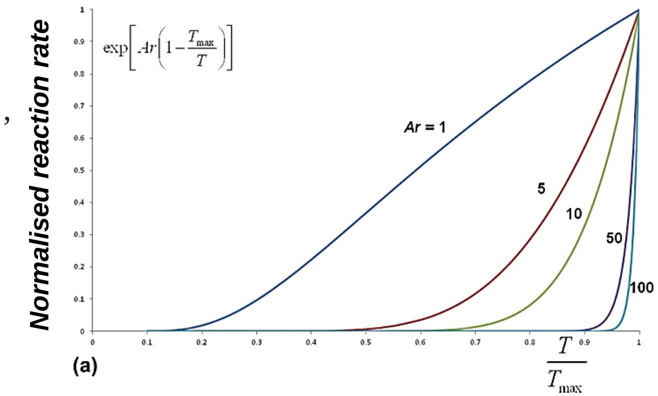
The larger the Arrhenius number, the more explosive and spatially localised the reaction is.

Activation energy

Arrhenius Number

$$Ar = \frac{E_a}{RT_{max}}$$

Maximum thermal in system energy



$$\text{Arrhenius Number, } Ar = \frac{\text{Activation energy, } E_a}{\text{Maximum thermal in system energy, } RT}$$

1. 5 diopside + anorthite + 4 H_2O + 6 CO_2 → chlorite + 9 quartz + 6 calcite; ΔH = -783.36 kJ,
2. 3 K–feldspar +2 H^+ → muscovite + 6 quartz +2K^+; ΔH = -485.23 kJ,
3. 6 actinolite +12 CO_2 + 14 H_2O → 5 chlorite + 12 calcite + 28 quartz; ΔH = +13,409.93 kJ,
4. $Au(HS)_2^- \rightarrow Au^+ + 2HS^-$ $\quad Au^+ + 0.5H_2 \rightarrow Au_{(solid)} + H^+$
5. $H_4SiO_4 \rightarrow SiO_{2(solid)} + 2H_2O$

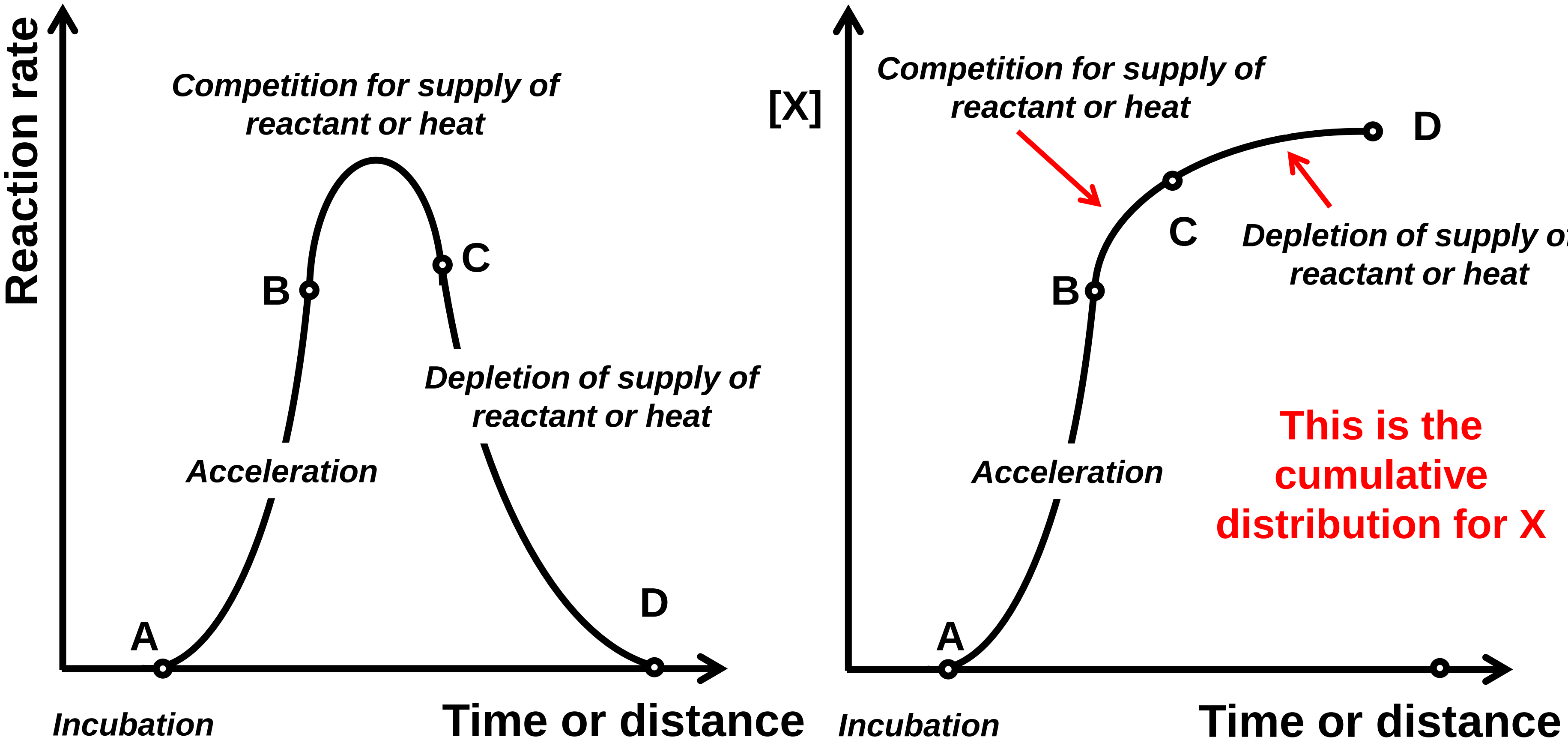
For T_{max} = 773K *Ar* is

1: 122
2: 75.5
3: 4173
4: 56
5: 11

Subcritical crack growth:
Ar = 3 - 15

Deposition of quartz is endothermic

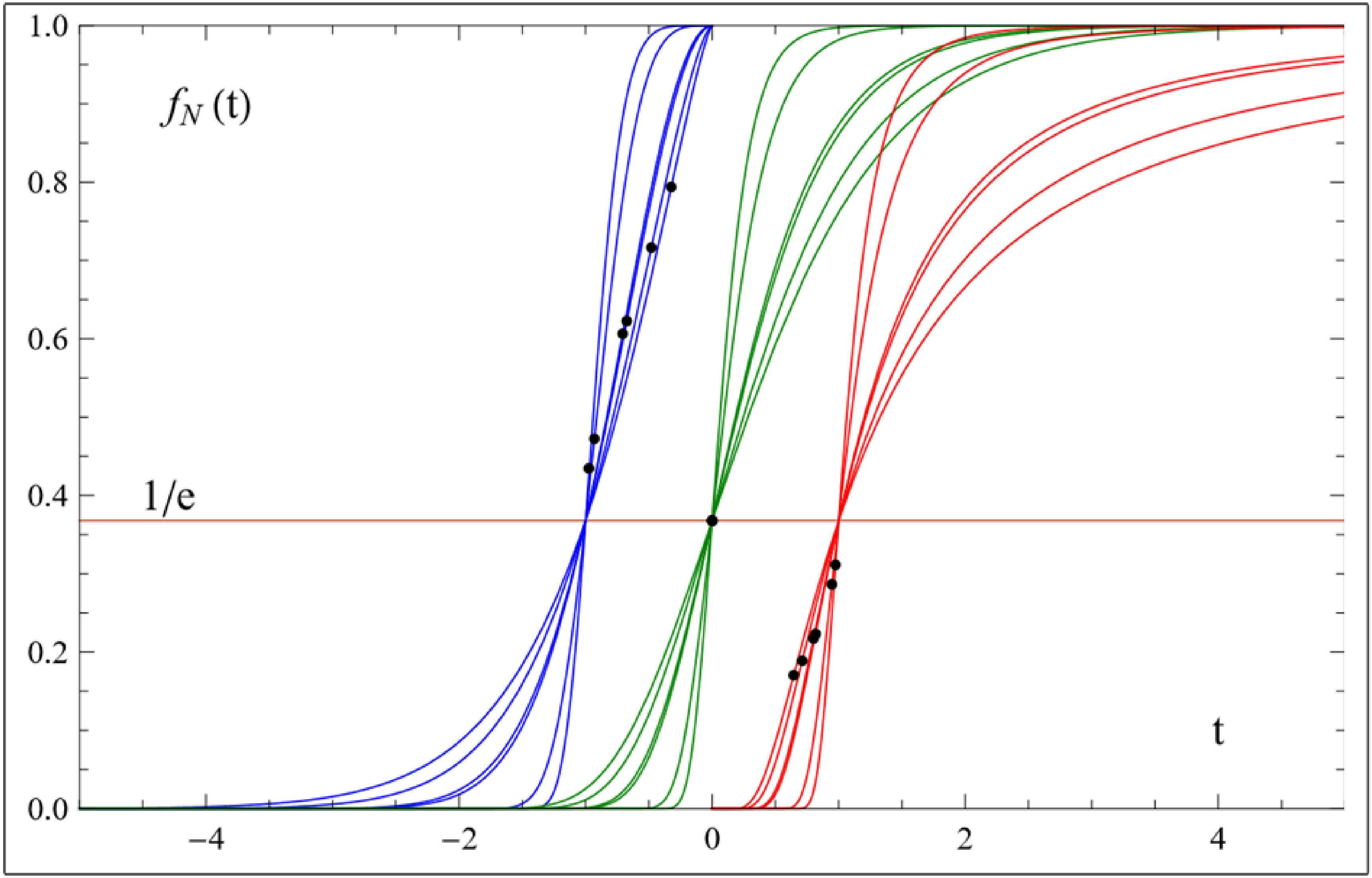
The history of an exothermal system



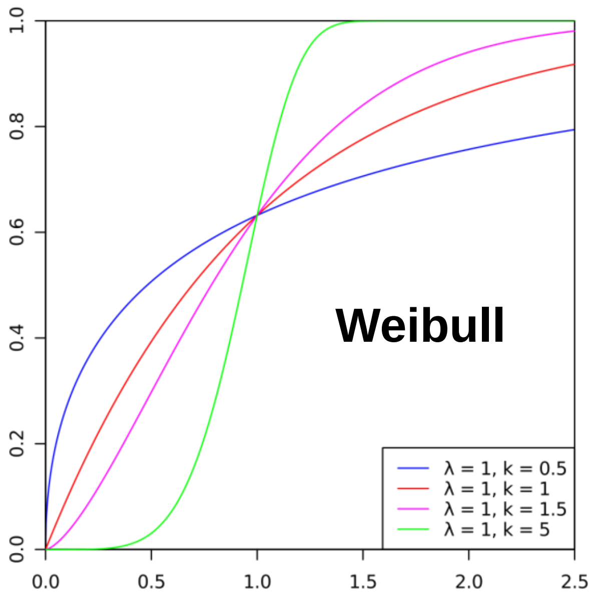
The precise shape of the cumulative distribution curve (and hence the endowment of the system) depends on the relative positions of A, B, C and D

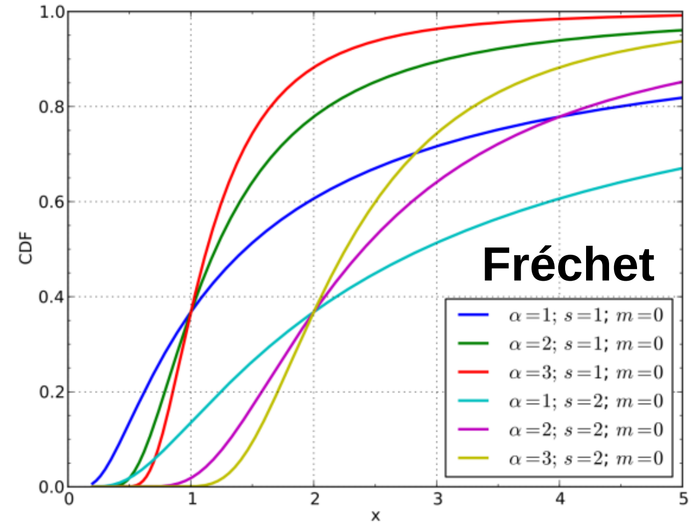
Nucleation → Growth controlled by supply of heat/mass → Extinction

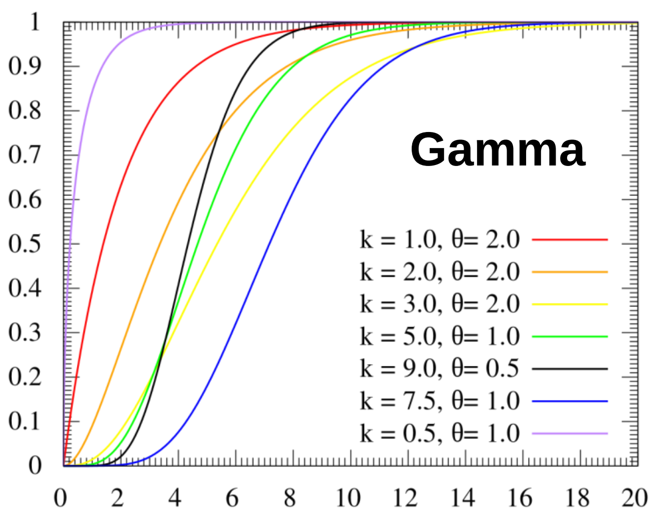
Leads to some form of sigmoidal growth curve

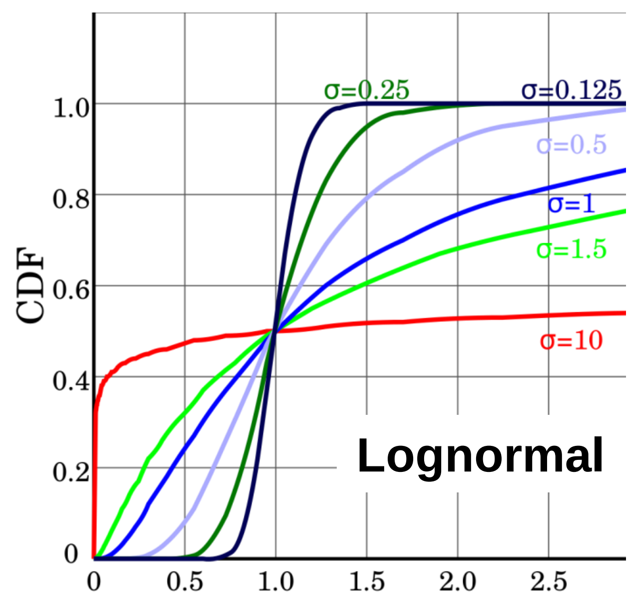


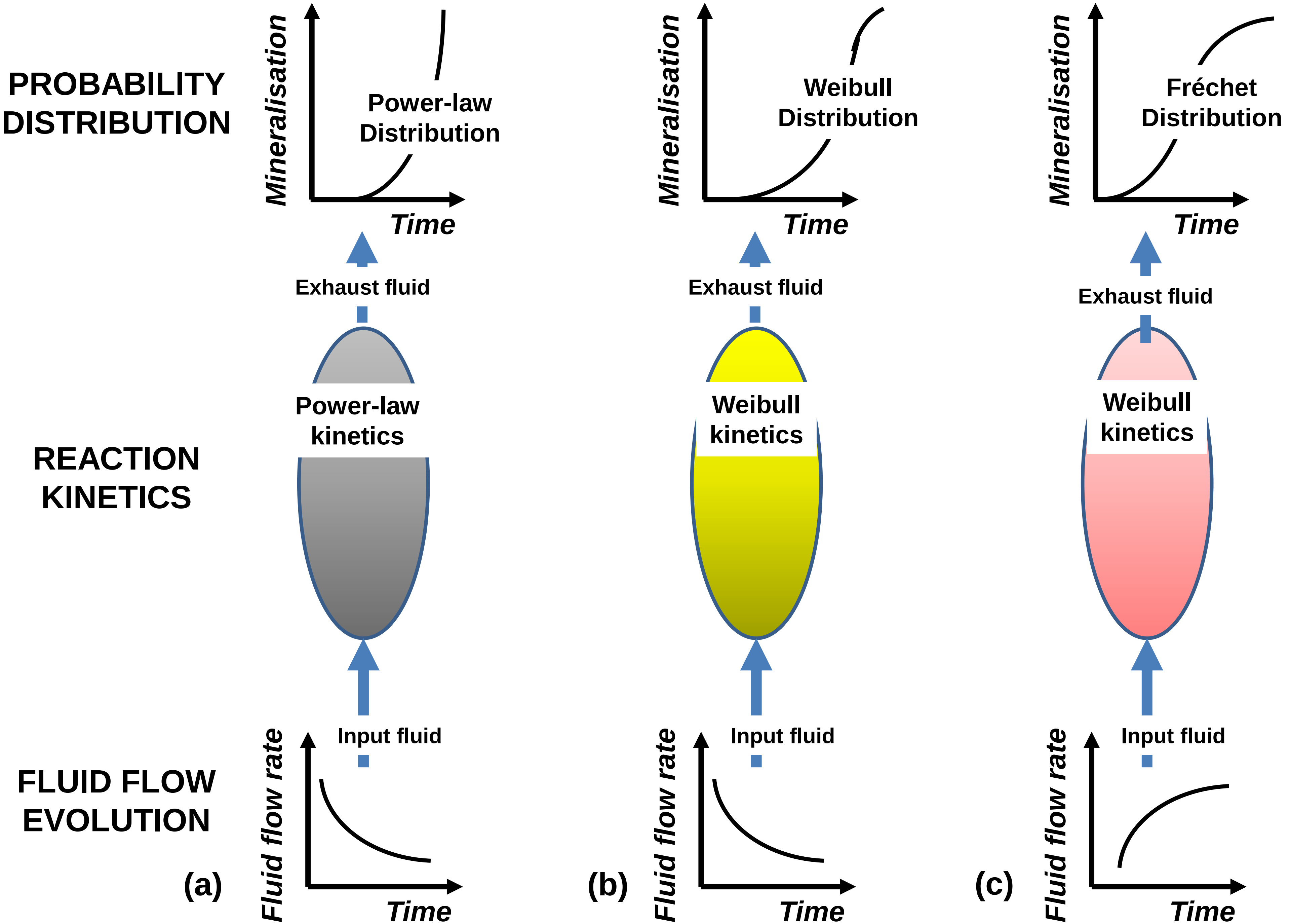
Four cumulative probability distributions of interest

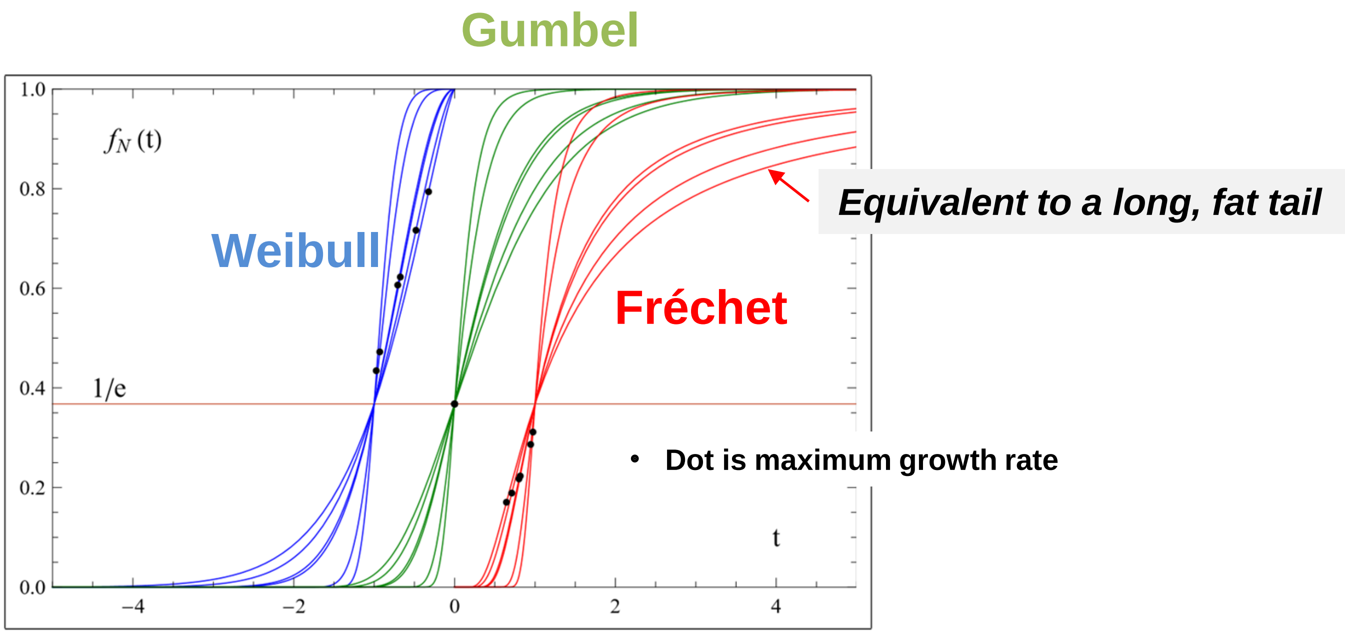









PROBABILITY DISTRIBUTION
REACTION KINETICS
FLUID FLOW EVOLUTION
(a)
Mineralisation
Power-law Distribution
Time
Exhaust fluid
Power-law kinetics
Input fluid
Fluid flow rate
Time
(b)
Mineralisation
Weibull Distribution
Time
Exhaust fluid
Weibull kinetics
Input fluid
Fluid flow rate
Time
(c)
Mineralisation
Fréchet Distribution
Time
Exhaust fluid
Weibull kinetics
Input fluid
Fluid flow rate
Time



Thus, systems that nucleate slowly, grow fast and die rapidly are likely to follow a Weibull distribution.

Systems that have a maximum growth rate exactly at 1/e are probably rare but correspond to Gumbel distributions.

Systems that nucleate rapidly and have variable growth rates but long lifetimes are likely to follow Fréchet distributions

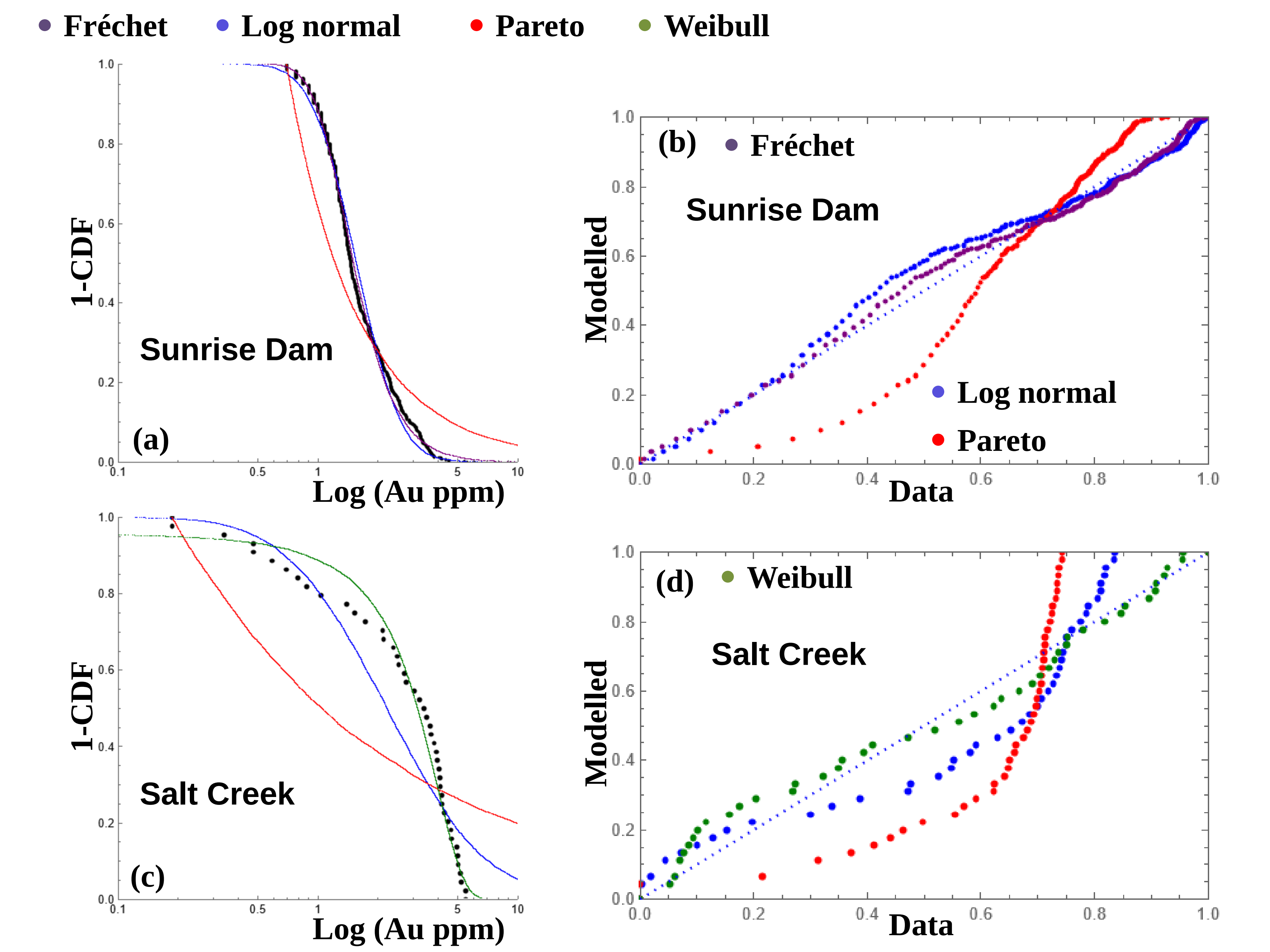
Thus we expect the cumulative probability distributions for mineral abundance and endowment to be some form of sigmoidal distribution.

This is true at all scales from regional to hand specimen scales.

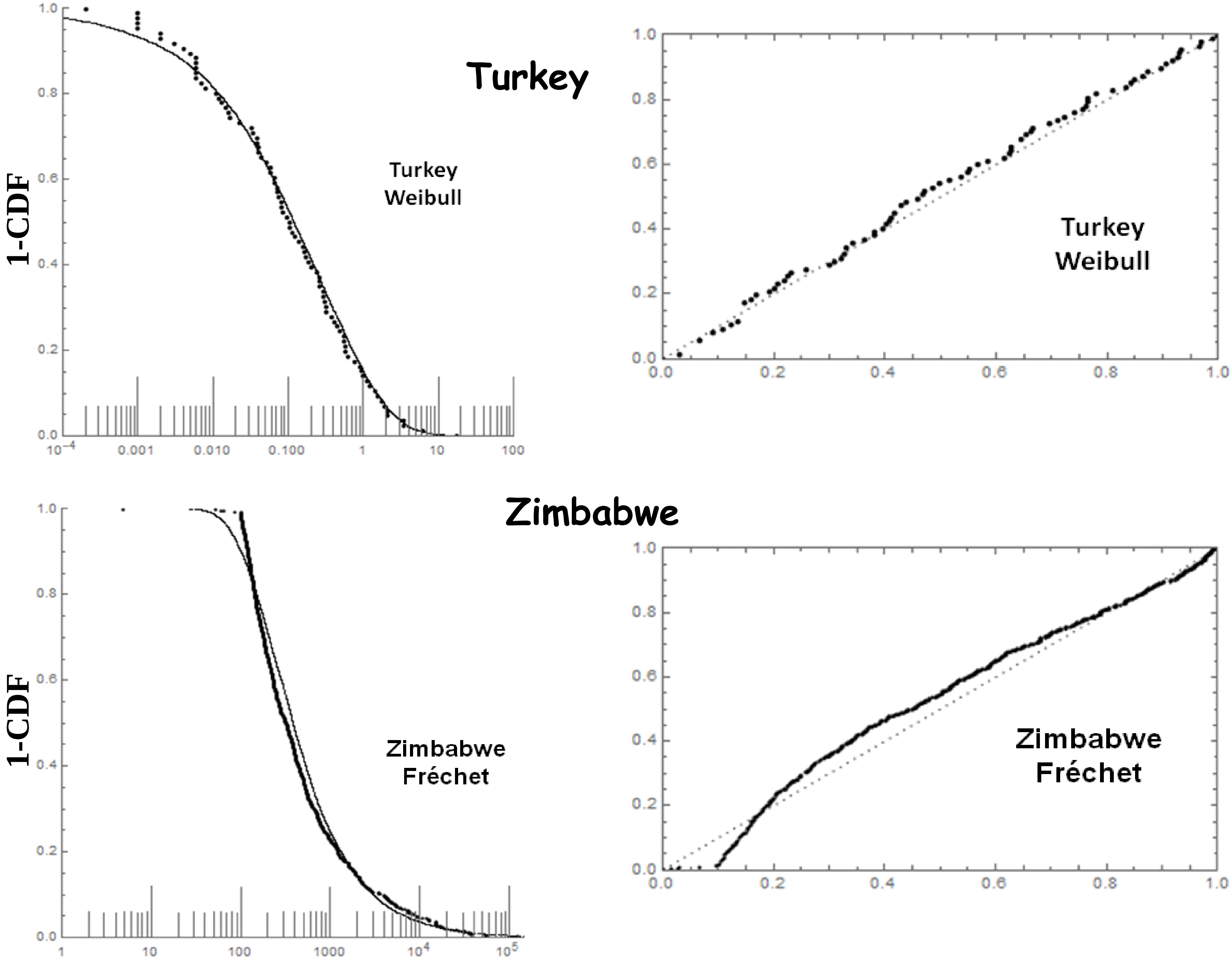
If a mineral system follows a common growth law throughout it will be characterised by a common cumulative probability distribution throughout.

Variations in the growth law at all scales are reflected in variations in the cumulative probability distribution at the various scales.

Ore body scale


Fréchet
Log normal
Pareto
Weibull
1-CDF
Sunrise Dam
(a)
Log (Au ppm)
(b)
Fréchet
Sunrise Dam
Modelled
Log normal
Pareto
Data
1-CDF
Salt Creek
(c)
Log (Au ppm)
(d)
Weibull
Salt Creek
Modelled
Data

Regional scale


Turkey
1-CDF
Turkey
Weibull
Turkey
Weibull
Zimbabwe
1-CDF
Zimbabwe
Fréchet
Zimbabwe
Fréchet

& indeed we observe the cumulative probability distributions for mineral abundance and endowment to be some form of sigmoidal distribution.

This is true at all scales from regional to hand specimen scales.

How further may we analyse the data?

Consider entropy.

Entropy says something about the quality of energy.

The first law of thermodynamics tells us that the amount of energy in the universe can never be depleted and nor will it grow.

For example, the energy stored in a log of wood is not lost when you ignite it. It just transfers into heat.

Just as two libraries contain the same number of books, they may differ in quality. In one library, all books are neatly arranged alphabetically on the bookshelves. In another we have a random-stacked pile. Although our two libraries contain the same number of books, they differ in the quality of service they can provide.

Consider entropy as a measure of quality of energy – the lower the entropy the higher the quality.

Energy stored in a carefully ordered way (the efficient library) has lower entropy. Energy stored in a chaotic way (the random-pile library) has high entropy.

the efficient library
lower entropy.

the random-pile library
higher entropy.

The link between probability and entropy.

If X is a continuous random variable with probability density p(x)
then the differential entropy of X is defined as

$$\boldsymbol{H}(\boldsymbol{X}) = -\int_{-\infty}^{\infty} \boldsymbol{p}(\boldsymbol{x})\mathbf{log}[\boldsymbol{p}(\boldsymbol{x})]\boldsymbol{d}\boldsymbol{x}$$

Entropy calculations for probability distributions

Gamma

sh shape parameter   sc scale parameter

Entropy = sh+Log[sc]+Log[Gamma[sh]]+(1-sh)*(Log[sh]-1/(2*sh))

LogNormal

mu mean   stdev standard deviation   of the normal distribution from which the lognormal distribution is derived

Entropy = Log[stdev*Exp[mu+0.5]*Sqrt[2*Pi]]

Frechet

alpha shape   sc scale   EulerGamma Eulers constant

Entropy=1+EulerGamma/alpha+EulerGamma+Log[sc/alpha]

The entropy tells us something about the shape of the distribution function.

Given two probability distributions defined over the same range, the broader, flatter distribution will have the larger entropy, a fact that is consistent with defining probability as a model for uncertainty.

We should be much less certain about the outcome of measurement modeled by a broad, flat distribution than we are about one governed by a distribution having a single sharp peak.

Two approaches to entropy

1. As a measure of uncertainty

2. As a measure of information

'in our practical experience, we have found the interpretation of entropy as uncertainty to be much more useful and much less prone to misunderstanding.

The larger the uncertainty about X, the larger the entropy associated with the probability distribution $p_X(x)$ of X.

Michalowicz et al. 2014   Handbook of Differential Entropy