GEOTRACES

An International Study of the Marine Biogeochemical Cycles of Trace Elements and their Isotopes

OCB

Ocean Carbon & Biogeochemistry

Modelling …

Alessandro Tagliabue

a.tagliabue@liverpool.ac.uk

UNIVERSITY OF LIVERPOOL

GEOTRACES / OCB Workshop 1-4 August 2016, Lamont

Overarching Goal

- Set the scene for discussion of how models may contribute to a better understanding of TEI internal cycling
  - How do models represent key TEI internal cycling processes?
  - What are their assumptions?
  - How can we make progress?

Disclaimer(s) …

- I will focus on:
  - General circulation style models
    - Nested within a physical framework
    - Important caveats associated with resolution
  - Models appropriate for decadal to centennial time scales
    - Resolving seasonality (resolving processes on hourly time scales)
    - Not box or inverse models
  - Processes relevant for bioactive TEs

So how do these models work?

```
         zTL1(ji,jj,jk) = ztotlig(ji,jj,jk)
         zkeq           = fekeq(ji,jj,jk)
         zfesatur       = zTL1(ji,jj,jk) * 1E-9
         ztfe           = trb(ji,jj,jk,jpfer)
         ! Fe' is the root of a 2nd order polynom
         zFe3 (ji,jj,jk) = ( -( 1. + zfesatur * zkeq - zkeq * ztfe )               &
            &              + SQRT( ( 1. + zfesatur * zkeq - zkeq * ztfe )**2       &
            &               + 4. * ztfe * zkeq) ) / ( 2. * zkeq )
         zFe3 (ji,jj,jk) = zFe3(ji,jj,jk) * 1E9
         zFeL1(ji,jj,jk) = MAX( 0., trb(ji,jj,jk,jpfer) * 1E9 - zFe3(ji,jj,jk) )
       END DO
     END DO
   END DO
   !
 ENDIF

 zdust = 0.         ! if no dust available
!CDIR NOVERRCHK
 DO jk = 1, jpkm1
!CDIR NOVERRCHK
   DO jj = 1, jpj
!CDIR NOVERRCHK
     DO ji = 1, jpi
       zstep = xstep
# if defined key_degrad
       zstep = zstep * facvol(ji,jj,jk)
# endif
       ! Scavenging rate of iron. This scavenging rate depends on the load of particles of sea water.
       ! This parameterization assumes a simple second order kinetics (k[Particles][Fe]).
       ! Scavenging onto dust is also included as evidenced from the DUNE experiments.
       ! --------------------------------------------------------------------------------------
       IF( ln_fechem ) THEN
          zfeequi = ( zFe3(ji,jj,jk) + zFe2(ji,jj,jk) + zFeP(ji,jj,jk) ) * 1E-9
          zfecoll = ( 0.3 * zFeL1(ji,jj,jk) + 0.5 * zFeL2(ji,jj,jk) ) * 1E-9
       ELSE
          IF (ln_fecolloid) THEN
             zfeequi = zFe3(ji,jj,jk) * 1E-9
             zhplus   = max( rtrn, hi(ji,jj,jk) )
             fe3sol  = fesol(ji,jj,jk)
!             fe3sol  = fesol(ji,jj,jk,1) * ( fesol(ji,jj,jk,2) * zhplus**2  &
!             &         + fesol(ji,jj,jk,3) * zhplus + fesol(ji,jj,jk,4)      &
!             &         + fesol(ji,jj,jk,5) / zhplus )
             zfecoll = max( ( 0.1 * zFeL1(ji,jj,jk) * 1E-9 ), ( zFeL1(ji,jj,jk) * 1E-9 -fe3sol ) )
          ELSE
             zfeequi = zFe3(ji,jj,jk) * 1E-9
             zfecoll = 0.5 * zFeL1(ji,jj,jk) * 1E-9
             fe3sol  = 0.
             kfep    = 0.
          ENDIF
       ENDIF
#if defined key_kriest
       ztrc   = ( trb(ji,jj,jk,jppoc) + trb(ji,jj,jk,jpcal) + trb(ji,jj,jk,jpgsi) ) * 1.e6
#else
       ztrc   = ( trb(ji,jj,jk,jppoc) + trb(ji,jj,jk,jpgoc) + trb(ji,jj,jk,jpcal) + trb(ji,jj,jk,jpgsi) ) * 1.e6
#endif
       IF( ln_dust )  zdust  = dust(ji,jj) / ( wdust / rday ) * tmask(ji,jj,jk) ! dust in kg/m2/s
       zlam1b = 3.e-5 + xlamdust * zdust + xlam1 * ztrc
       zscave = zfeequi * zlam1b * zstep

       ! Compute the different ratios for scavenging of iron
       ! to later allocate scavenged iron to the different organic pools
       ! ---------------------------------------------------------
       zdenom1 = xlam1 * trb(ji,jj,jk,jppoc) / zlam1b
#if ! defined key_kriest
       zdenom2 = xlam1 * trb(ji,jj,jk,jpgoc) / zlam1b
```

```
         ! Compute the proportion of filter feeders
         zproport  = (zgrazffep + zgrazffeg)/(rtrn + zgraztot)
         ! Compute fractionation of aggregates. It is assumed that
         ! diatoms based aggregates are more prone to fractionation
         ! since they are more porous (marine snow instead of fecal pellets)
         zratio    = trb(ji,jj,jk,jpgsi) / ( trb(ji,jj,jk,jpgoc) + rtrn )
         zratio2   = zratio * zratio
         zfrac     = zproport * grazflux  * zstep * wsbio4(ji,jj,jk)      &
          &          * trb(ji,jj,jk,jpgoc) * trb(ji,jj,jk,jpmes)          &
          &          * ( 0.2 + 3.8 * zratio2 / ( 1.**2 + zratio2 ) )
         zfracfe   = zfrac * trb(ji,jj,jk,jpbfe) / (trb(ji,jj,jk,jpgoc) + rtrn)

         zgrazffep = zproport * zgrazffep
         zgrazffeg = zproport * zgrazffeg
         zgrazfffp = zproport * zgrazfffp
         zgrazfffg = zproport * zgrazfffg
         zgraztot  = zgrazd + zgrazz + zgrazn + zgrazpoc + zgrazffep + zgrazffeg
         zgraztotn = zgrazd * quotad(ji,jj,jk) + zgrazz + zgrazn * quotan(ji,jj,jk)   &
         &   + zgrazpoc + zgrazffep + zgrazffeg
         zgraztotf = zgrazf + zgraznf + zgrazz * ferat3 + zgrazpof + zgrazfffp + zgrazfffg
# else
         zgraztot  = zgrazd + zgrazz + zgrazn + zgrazpoc + zgrazffep
         ! Compute the proportion of filter feeders
         zproport  = zgrazffep / ( zgraztot + rtrn )
         zgrazffep = zproport * zgrazffep
         zgrazfffp = zproport * zgrazfffp
         zgraztot  = zgrazd + zgrazz + zgrazn + zgrazpoc + zgrazffep
         zgraztotn = zgrazd * quotad(ji,jj,jk) + zgrazz + zgrazn * quotan(ji,jj,jk) + zgrazpoc + zgrazffep
         zgraztotf = zgrazf + zgraznf + zgrazz * ferat3 + zgrazpof + zgrazfffp
# endif

         ! Total grazing ( grazing by microzoo is already computed in p4zmicro )
         IF( lk_iomput )  zgrazing(ji,jj,jk) = zgraztot

         !    Mesozooplankton efficiency
         !    ---------------------------
          zgrasrat  =  ( zgraztotf +rtrn )/ ( zgraztot + rtrn )
          zgrasratn =  ( zgraztotn +rtrn )/ ( zgraztot + rtrn )
          zepshert  = MIN( 1., zgrasratn, zgrasrat / ferat3)
          zepsherv  = zepshert * MIN( epsher2, (1. - unass2) * zgrasrat / ferat3, (1. - unass2) * zgrasratn )
          zgrarem2  = zgraztot * ( 1. - zepsherv - unass2 ) &
           &       + ( 1. - epsher2 - unass2 ) / ( 1. - epsher2 ) * ztortz2
          zgrafer2  = zgraztot * MAX( 0. , ( 1. - unass2 ) * zgrasrat - ferat3 * zepsherv )    &
           &       + ferat3 * ( ( 1. - epsher2 - unass2 ) /( 1. - epsher2 ) * ztortz2 )
          zgrapoc2  = zgraztot * unass2

          !   Update the arrays TRA which contain the biological sources and sinks
          zgrarsig  = zgrarem2 * sigma2
          tra(ji,jj,jk,jppo4) = tra(ji,jj,jk,jppo4) + zgrarsig
          tra(ji,jj,jk,jpnh4) = tra(ji,jj,jk,jpnh4) + zgrarsig
          tra(ji,jj,jk,jpdoc) = tra(ji,jj,jk,jpdoc) + zgrarem2 - zgrarsig
#if defined key_ligand
          tra(ji,jj,jk,jplgw) = tra(ji,jj,jk,jplgw) + (zgrarem2 - zgrarsig) * ldocz
          zz2ligprod(ji,jj,jk) = (zgrarem2 - zgrarsig) * ldocz
#endif
          tra(ji,jj,jk,jpoxy) = tra(ji,jj,jk,jpoxy) - o2ut * zgrarsig
          tra(ji,jj,jk,jpfer) = tra(ji,jj,jk,jpfer) + zgrafer2
          zfezoo2(ji,jj,jk) = zgrafer2
          tra(ji,jj,jk,jpdic) = tra(ji,jj,jk,jpdic) + zgrarsig
          tra(ji,jj,jk,jptal) = tra(ji,jj,jk,jptal) + rno3 * zgrarsig

          zmortz2 = ztortz2 + zrespz2
          zmortzgoc = unass2 / ( 1. - epsher2 ) * ztortz2 + zrespz2
          tra(ji,jj,jk,jpmes) = tra(ji,jj,jk,jpmes) - zmortz2 + zepsherv * zgraztot
          tra(ji,jj,jk,jpdia) = tra(ji,jj,jk,jpdia) - zgrazd
```

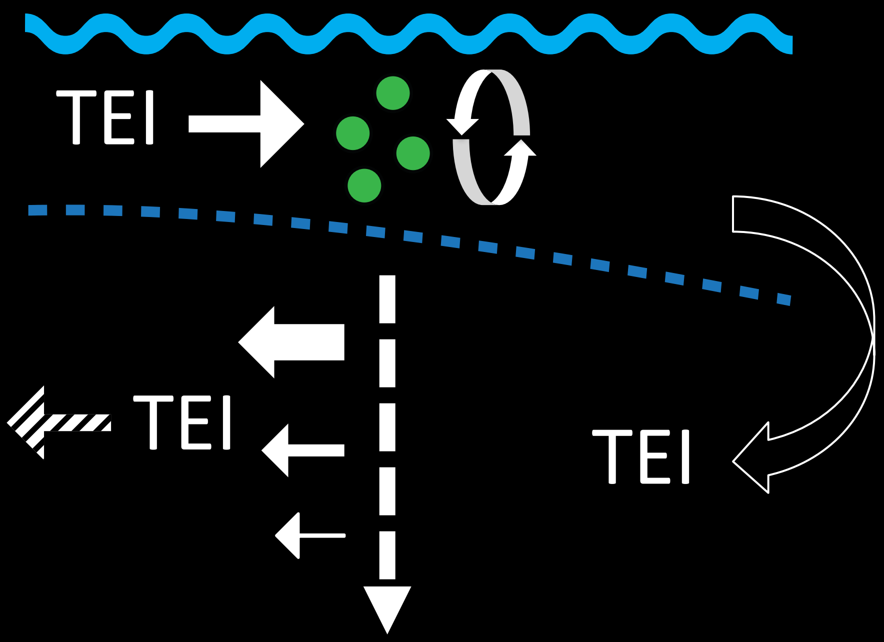
What are the main processes at play?

Surface uptake and cycling

Sinking and regeneration

Scavenging

Subduction and transport



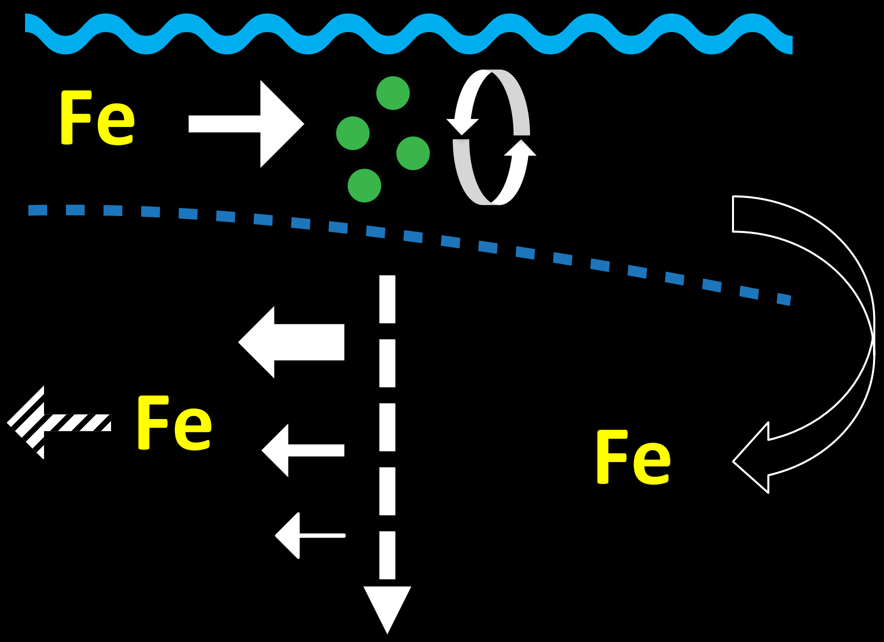
What are the main processes at play?

Surface uptake and cycling

~~Sinking and~~ regeneration

Scavenging

Subduction and transport

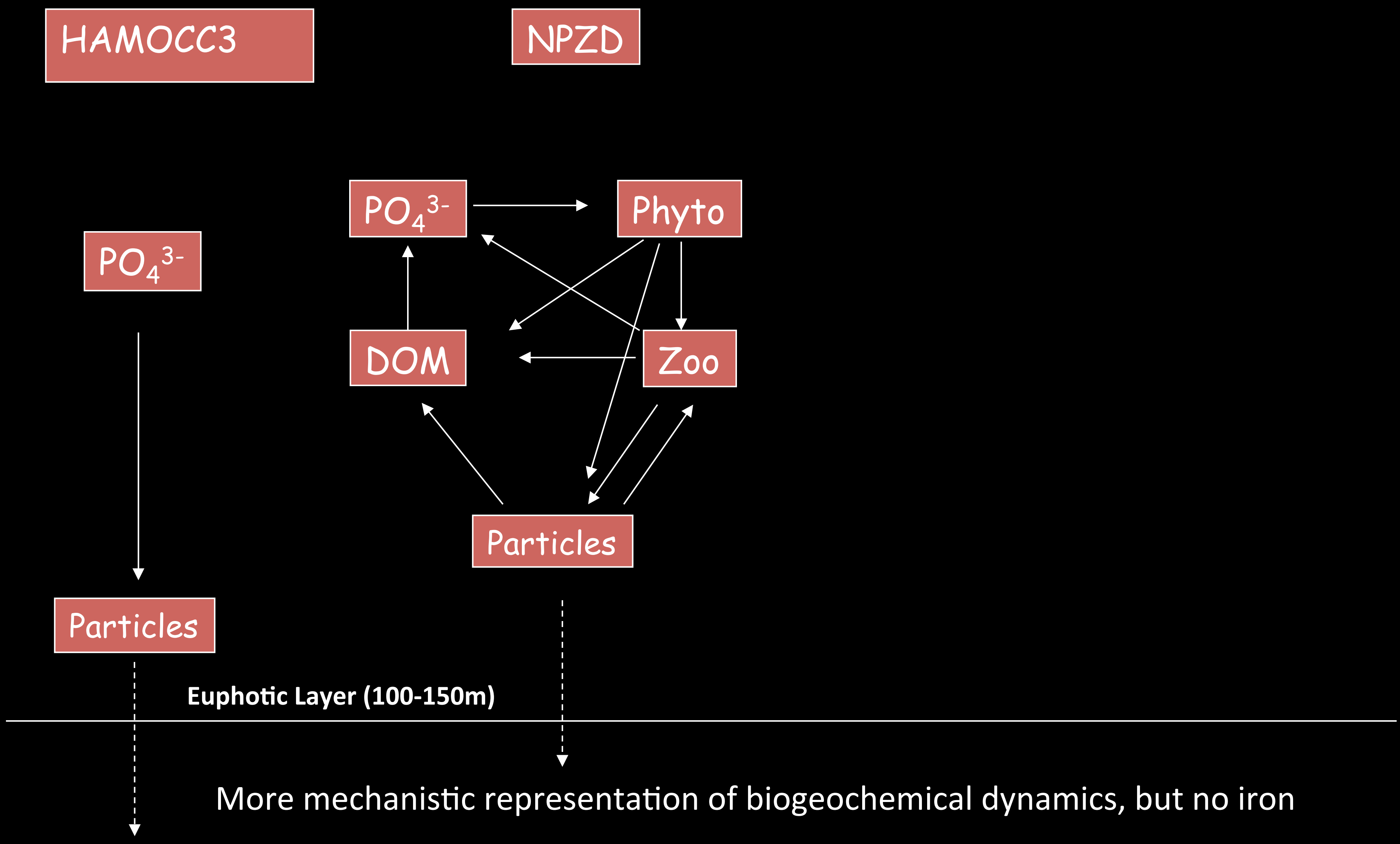


Necessary focus here on Fe …

Evolution of internal cycling in GCMs

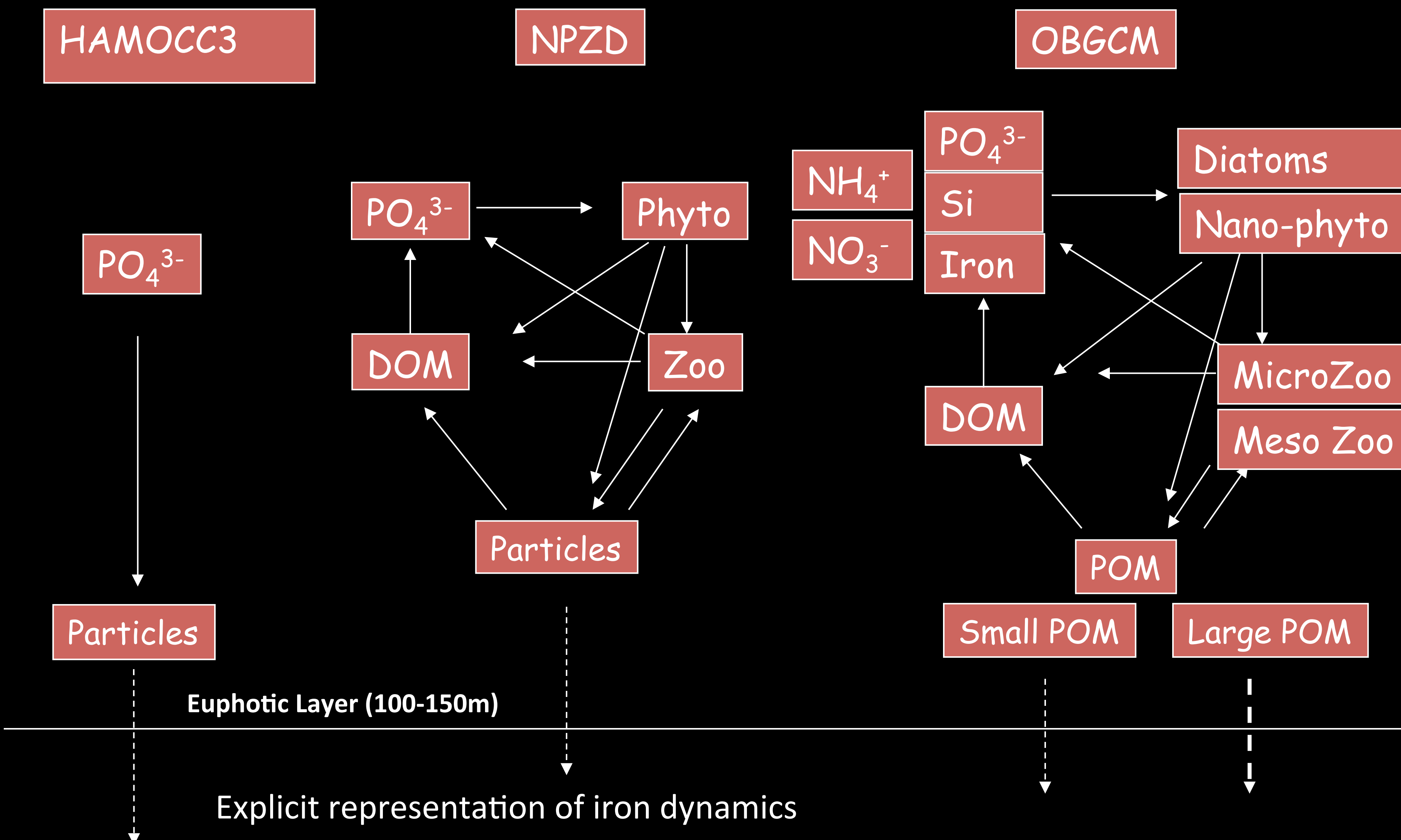
Effect of iron could only be assessed implicitly (cf. early iron fertlisation studies)

Evolution of internal cycling in GCMs

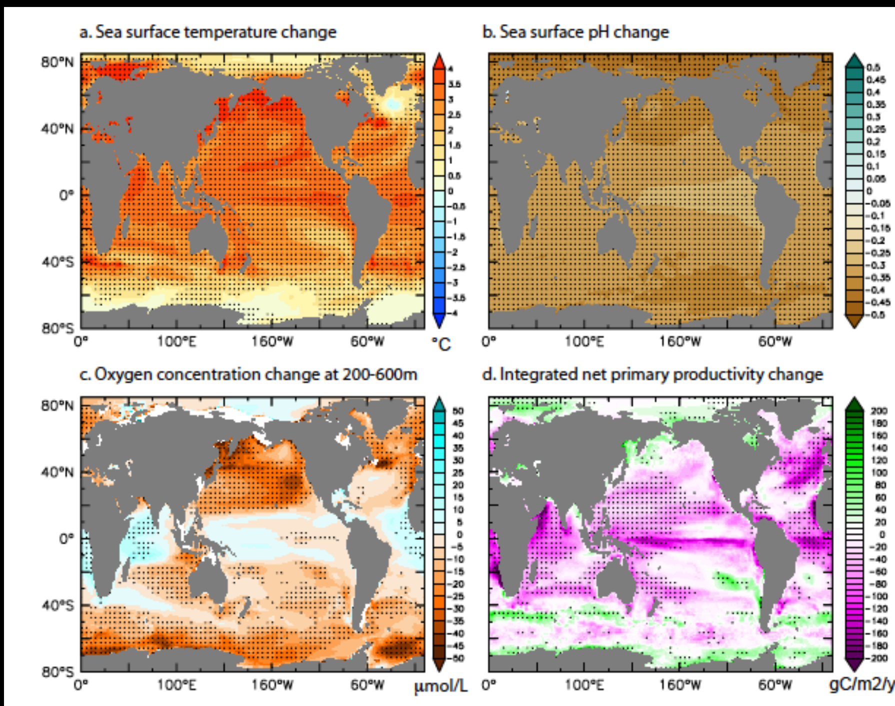


More mechanistic representation of biogeochemical dynamics, but no iron

Evolution of internal cycling in GCMs



We rely on models …

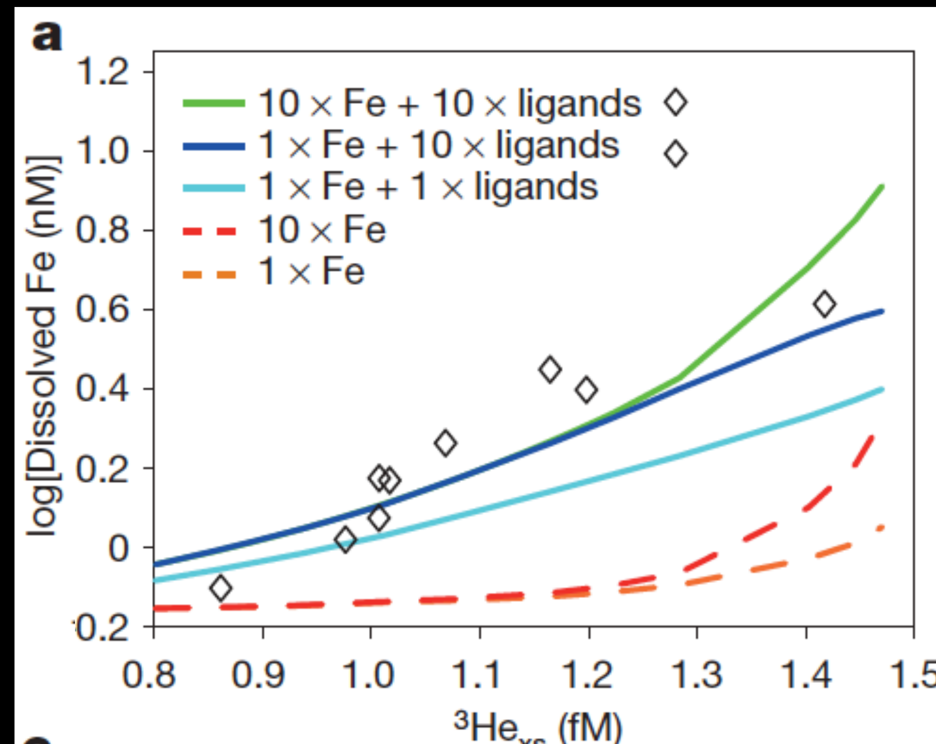


Biogeosciences, 10, 6225–6245, 2013
www.biogeosciences.net/10/6225/2013/
doi:10.5194/bg-10-6225-2013

Biogeosciences Open Access

Multiple stressors of ocean ecosystems in the 21st century: projections with CMIP5 models

L. Bopp[1], L. Resplandy[1], J. C. Orr[1], S. C. Doney[8], J. P. Dunne[2], M. Gehlen[1], P. Halloran[3], C. Heinze[6,9,10], T. Ilyina[4], R. Séférian[1,5], J. Tjiputra[6,9,10], and M. Vichi[7]



LETTER

doi:10.1038/nature14577

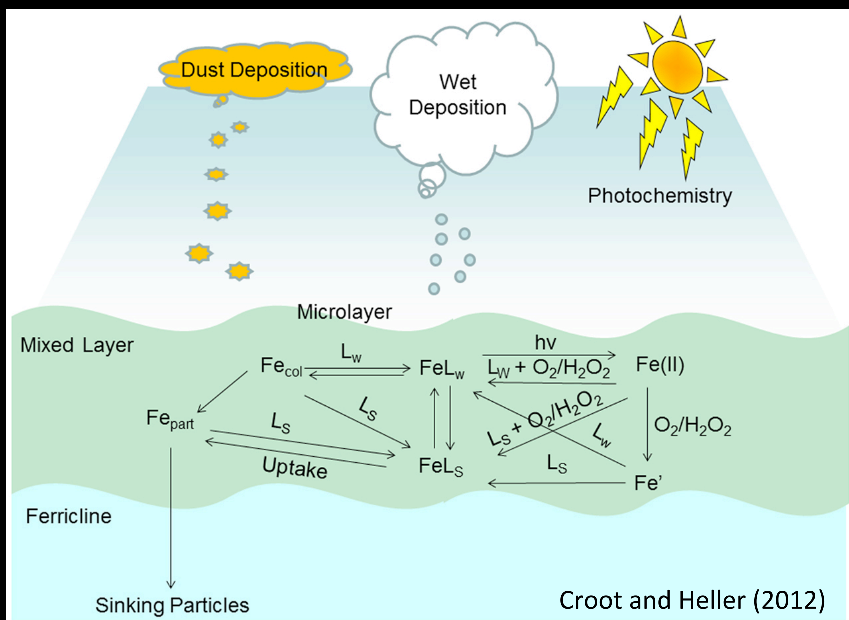
Basin-scale transport of hydrothermal dissolved metals across the South Pacific Ocean

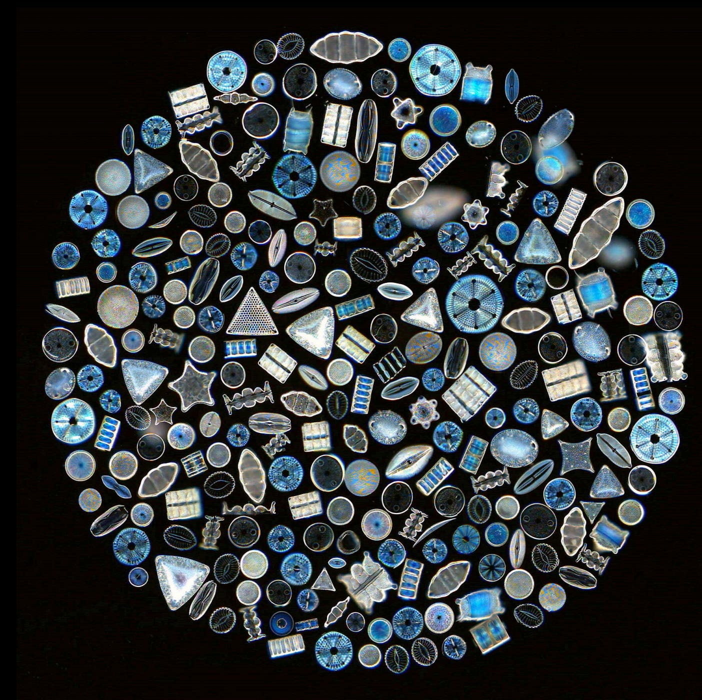
Joseph A. Resing[1], Peter N. Sedwick[2], Christopher R. German[3], William J. Jenkins[3], James W. Moffett[4], Bettina M. Sohst[2] & Alessandro Tagliabue[5]

Projecting the future **Testing hypotheses**

Models are underpinned by *trade offs*

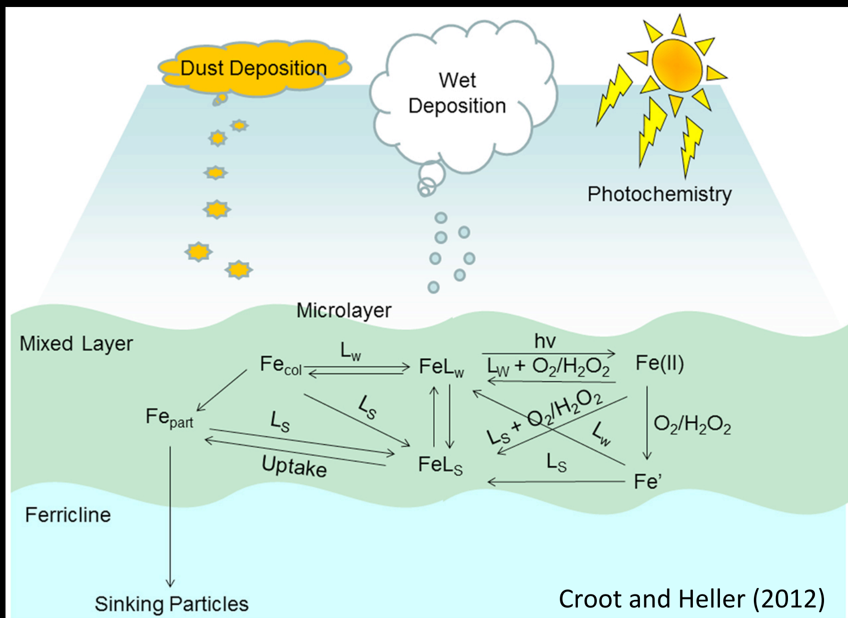
- We *want* lots of processes to reflect the complexity of nature …

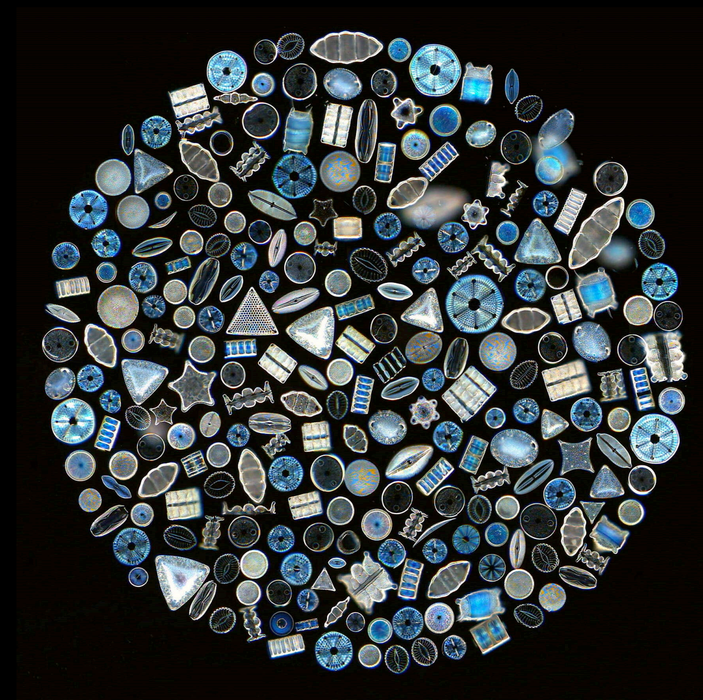




Models are underpinned by *trade offs*

- We *want* lots of processes to reflect the complexity of nature …





- But we face two trade offs:
  - How do we parameterise the model?
  - It may become too slow to be useful

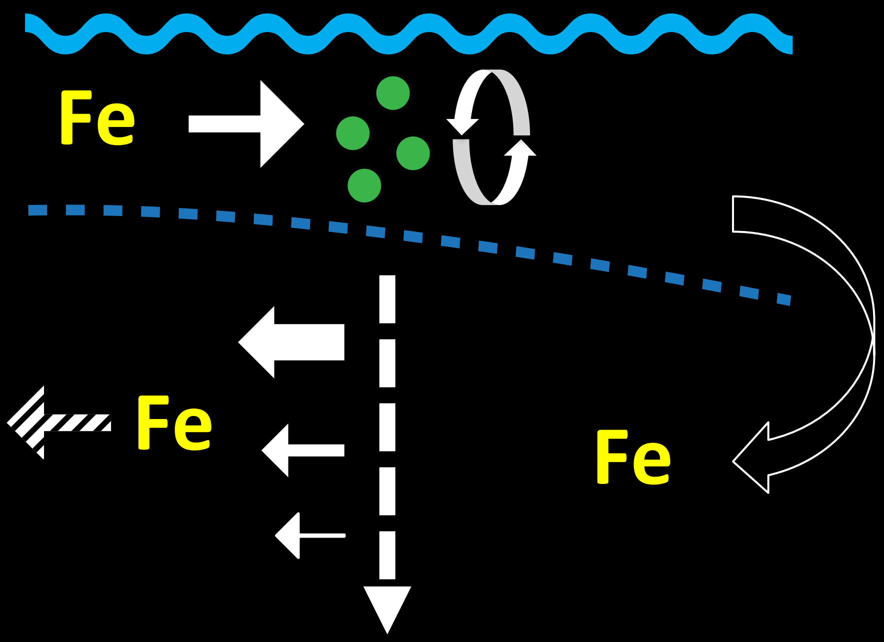
What are the main processes at play?

Surface uptake and cycling

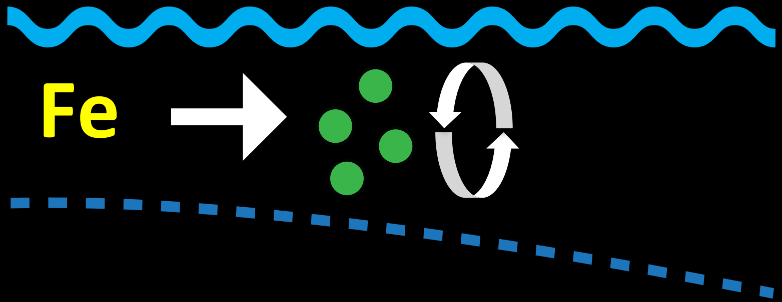
~~Sinking and~~ regeneration

Scavenging

Subduction and transport

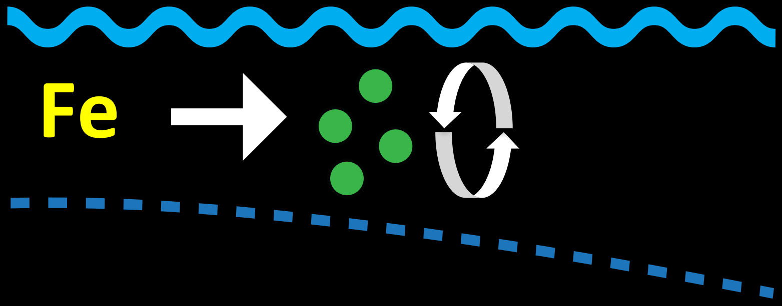


Surface uptake and cycling



Three main concepts to deal with:

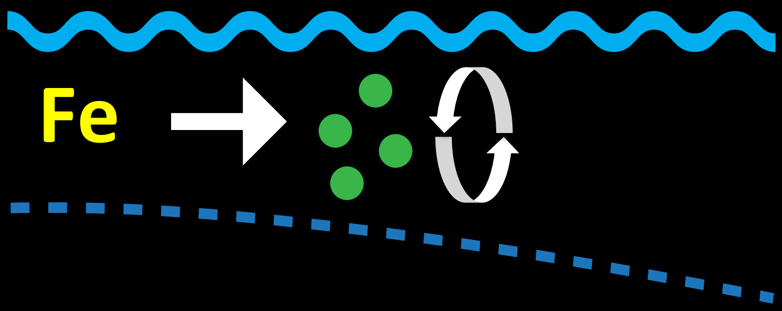
Surface uptake and cycling



Three main concepts to deal with:

1. Uptake
2. Impact on Growth rate
3. Recycling

Surface uptake and cycling

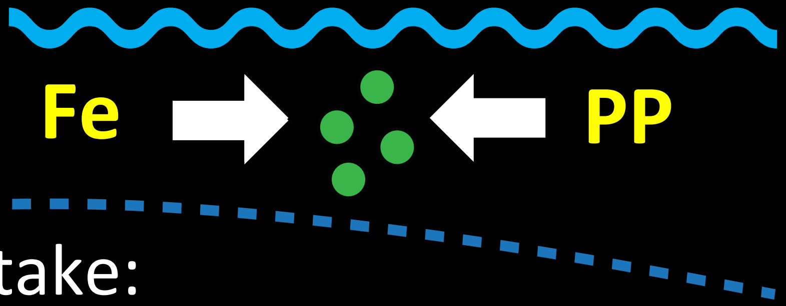


Three main concepts to deal with:

1. **Uptake**
2. Impact on Growth rate
3. Recycling

Uptake by microbes

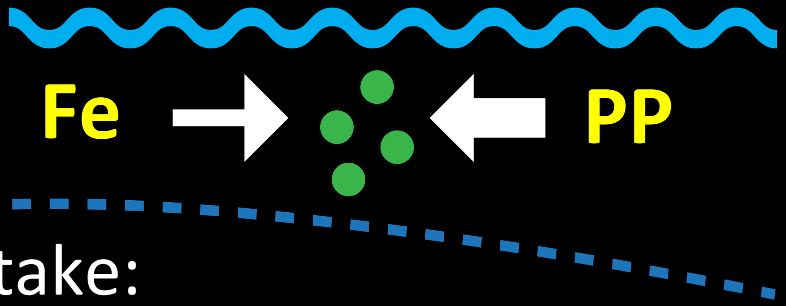
Two main philosophies



1. **Coupled** (aka "Redfield") uptake:

Fe uptake derived from rate of primary production via imposed stoichiometry:

Uptake by microbes



Two main philosophies

1. **Coupled** (aka "Redfield") uptake:

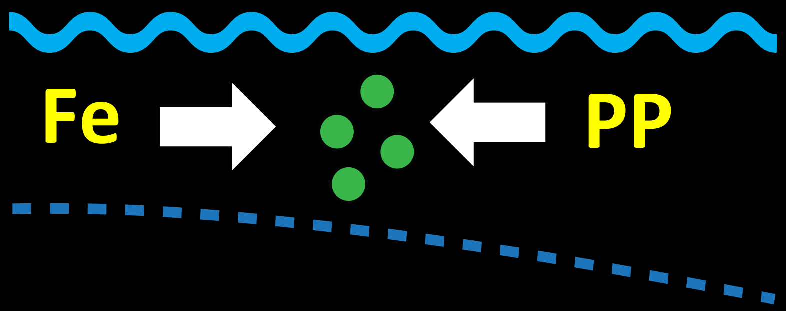
Fe uptake derived from rate of primary production via imposed stoichiometry

2. **Decoupled** (aka "Michaelis Menten") uptake:

Fe uptake derived independent of primary production via kinetic equations

“Coupled” uptake by microbes

Main assumptions:



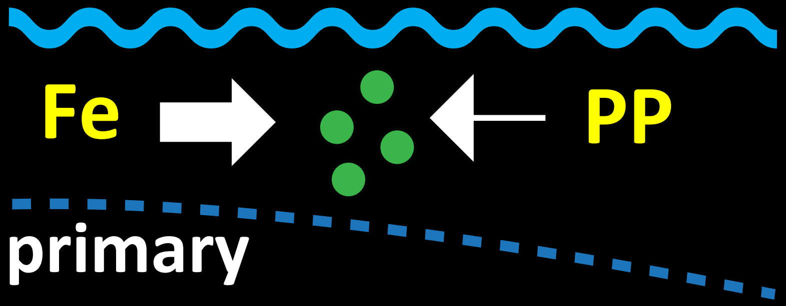
- Uptake of Fe is ‘slave’ to primary production

- Often driven by fixed Fe/C stoichiometry

-> Fe uptake varies proportionally with PP and growth

-> Fixed Fe/C stoichiometry attractive from an efficiency standpoint (cf. trade offs)

“Decoupled” uptake by microbes



Main assumptions:

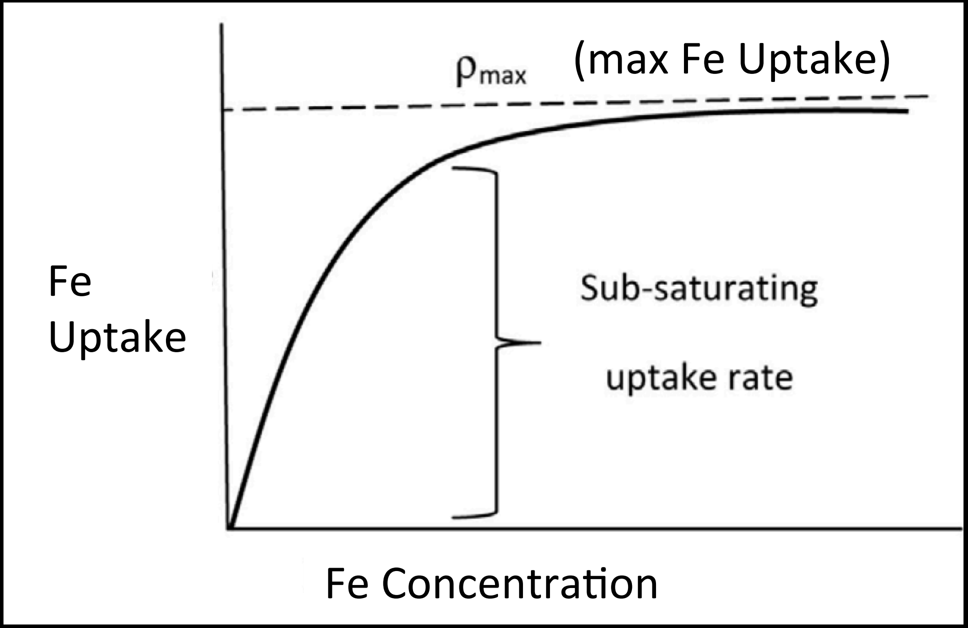
- Uptake of Fe is independent of primary production

- Driven by Michaelis Menten Kinetics

-> Allows Fe uptake to continue when PP is limited (e.g. by light)

-> More computationally expensive

“Decoupled” uptake by microbes



Adapted from Shaked and Lis (2012)

$$\rho = \rho_{MAX} \frac{Fe}{Fe + K_s} + \textbf{Luxury} + \textbf{Surge}$$

sensu Morel (1987, J Phyc)

“Decoupled” uptake by microbes

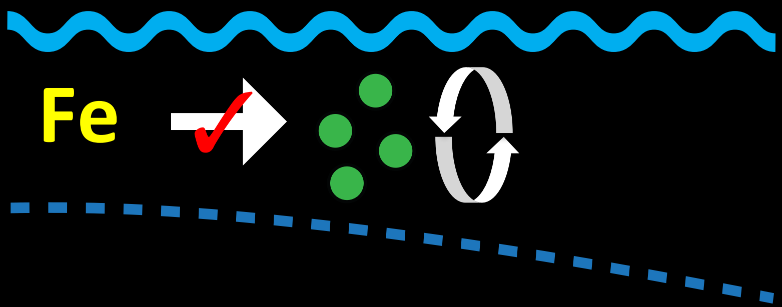
Key parameters:

- Affinity for (specific?) forms of Fe

- Imposed maximum cellular quota

- Relative increase in Fe uptake at low Fe

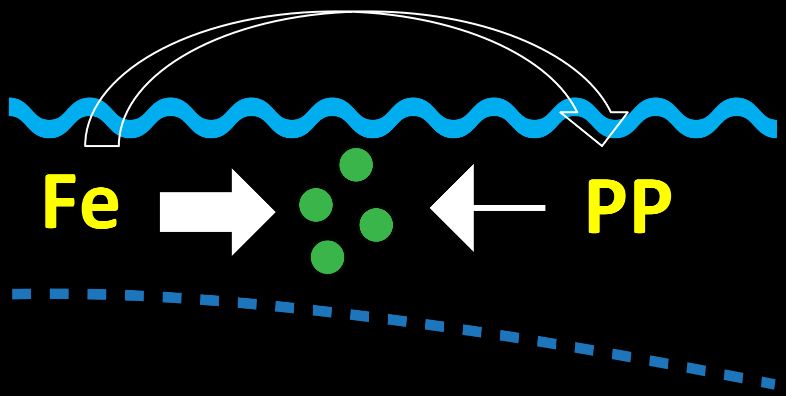
Surface uptake and cycling



Three main concepts to deal with:

1. Uptake
2. **Impact on Growth rate**
3. Recycling

Growth Limitation



Two main philosophies

1. Monod Limitation:

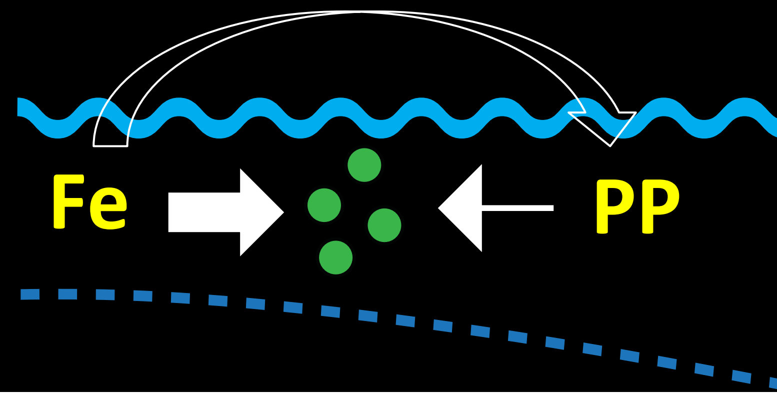
Simplest ; external concentration drives growth rate

2. Quota (or Droop) Limitation:

Complex ; internal quota drives growth rate

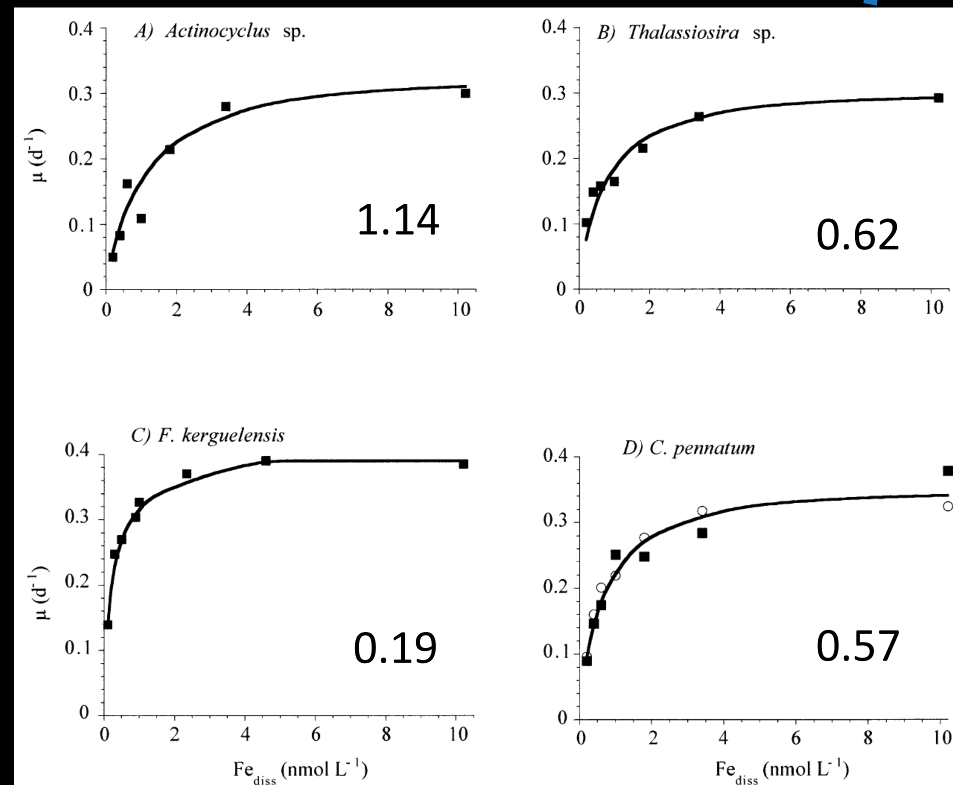
Growth Limitation

Two main philosophies



1. Monod Limitation:

$$\mu = \mu_{MAX} \frac{Fe}{Fe + K_{\mu}}$$

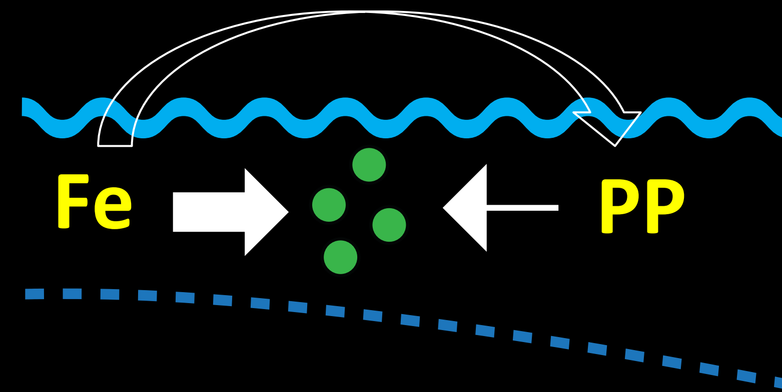


Key parameter is K_{μ} ; can be derived from experimental studies

Timmermans et al (2004, L&O)

Growth Limitation

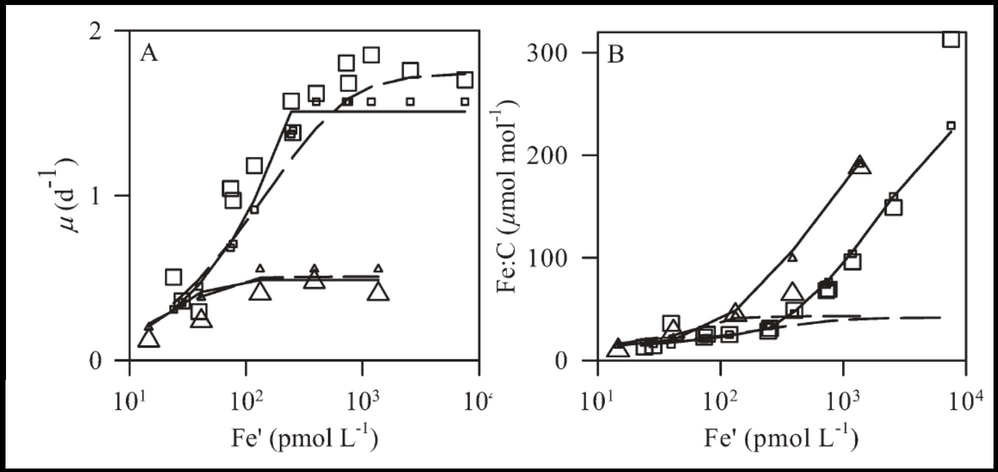
Two main philosophies



2. Quota Limitation

$$\mu = \mu_{MAX} \frac{Q - Q_{REQ}}{Q_{OPT}}$$

Key parameters are **Q_{REQ} and Q_{OPT}**; can be derived from first principles / physiology / optimisation



Buitenhuis and Geider (2010, L&O)

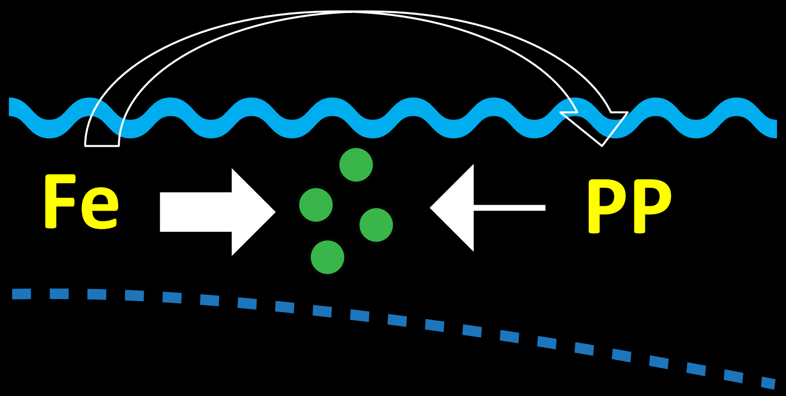
Growth Limitation

Two main philosophies

2. Quota Limitation

$$\mu = \mu_{MAX} \frac{Q - Q_{REQ}}{Q_{OPT}}$$

Key parameters are **Q_{REQ} and Q_{OPT}**; can be derived from **first principles** / physiology / optimisation



Contributions from:

Fe/Chl per PSU

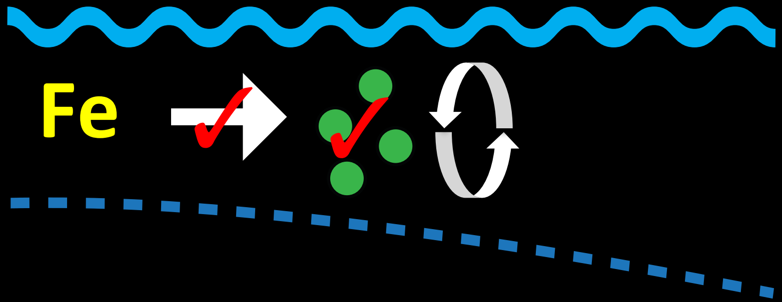
Nitrate reduction

Respiration

Provides mechanistic links to physiology!

after Raven (1990, J Phyc) Flynn and Hipkin (1999, JPR)

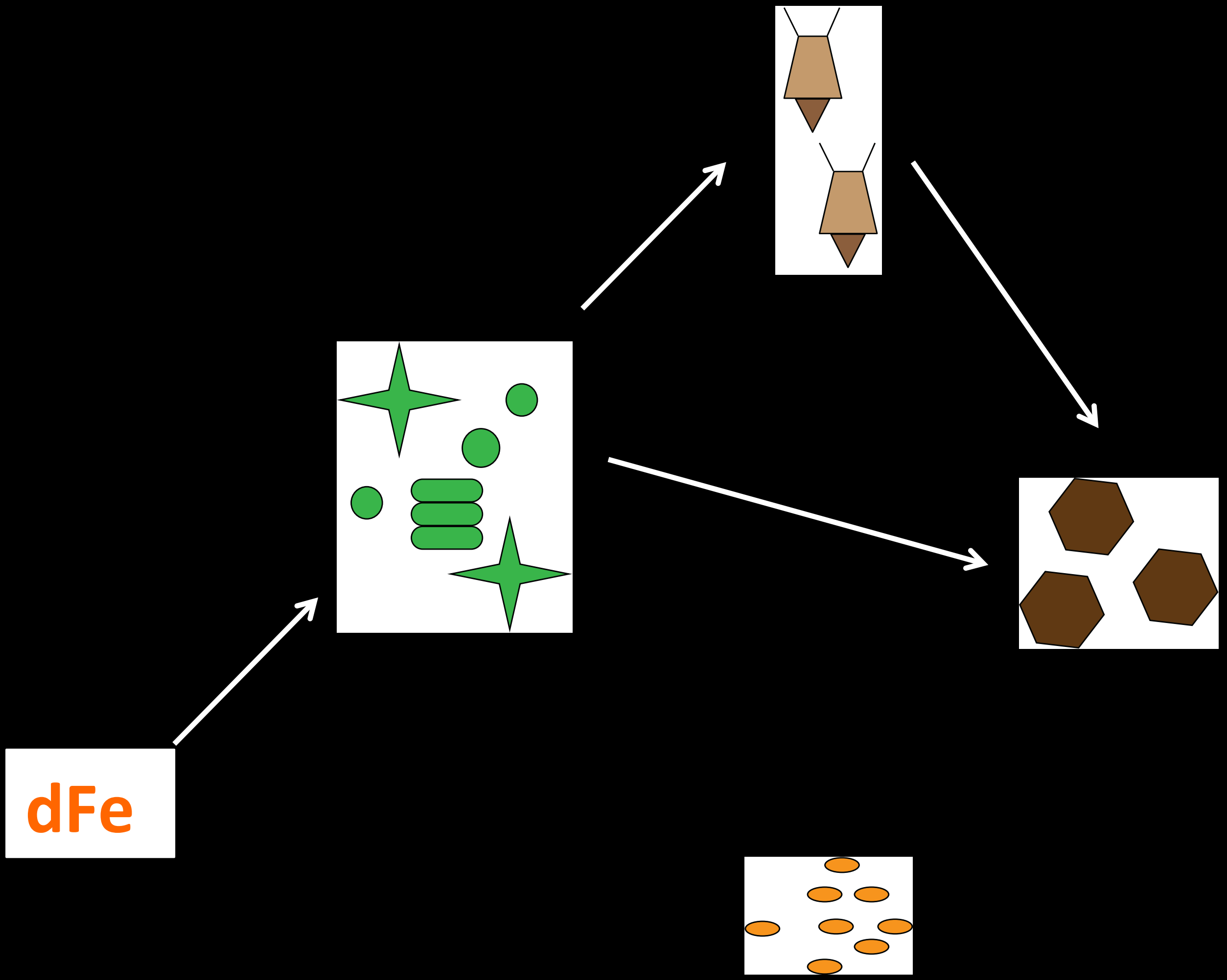
Surface uptake and cycling



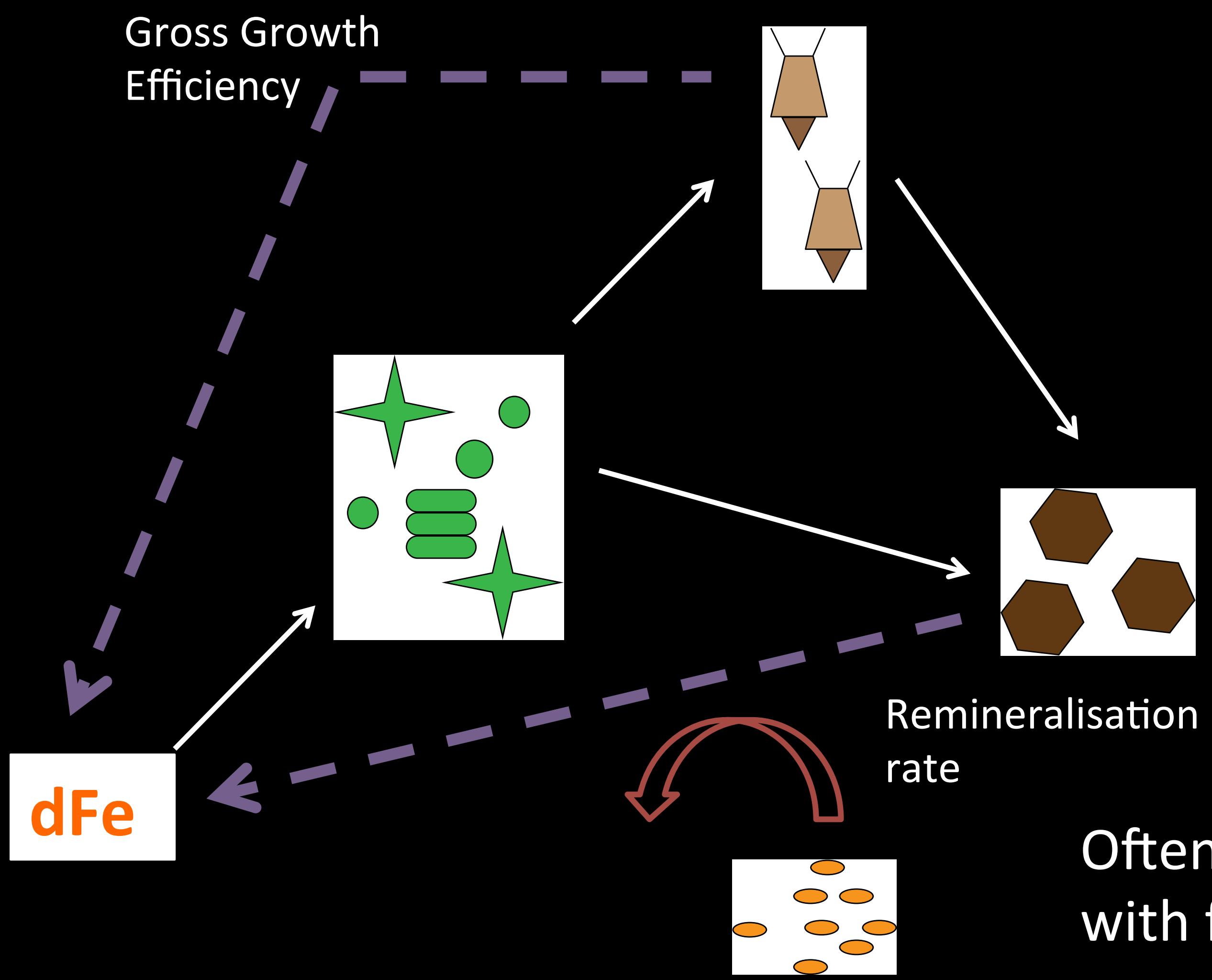
Three main concepts to deal with:

1. Uptake
2. Impact on Growth rate
3. **Recycling**

Recycling

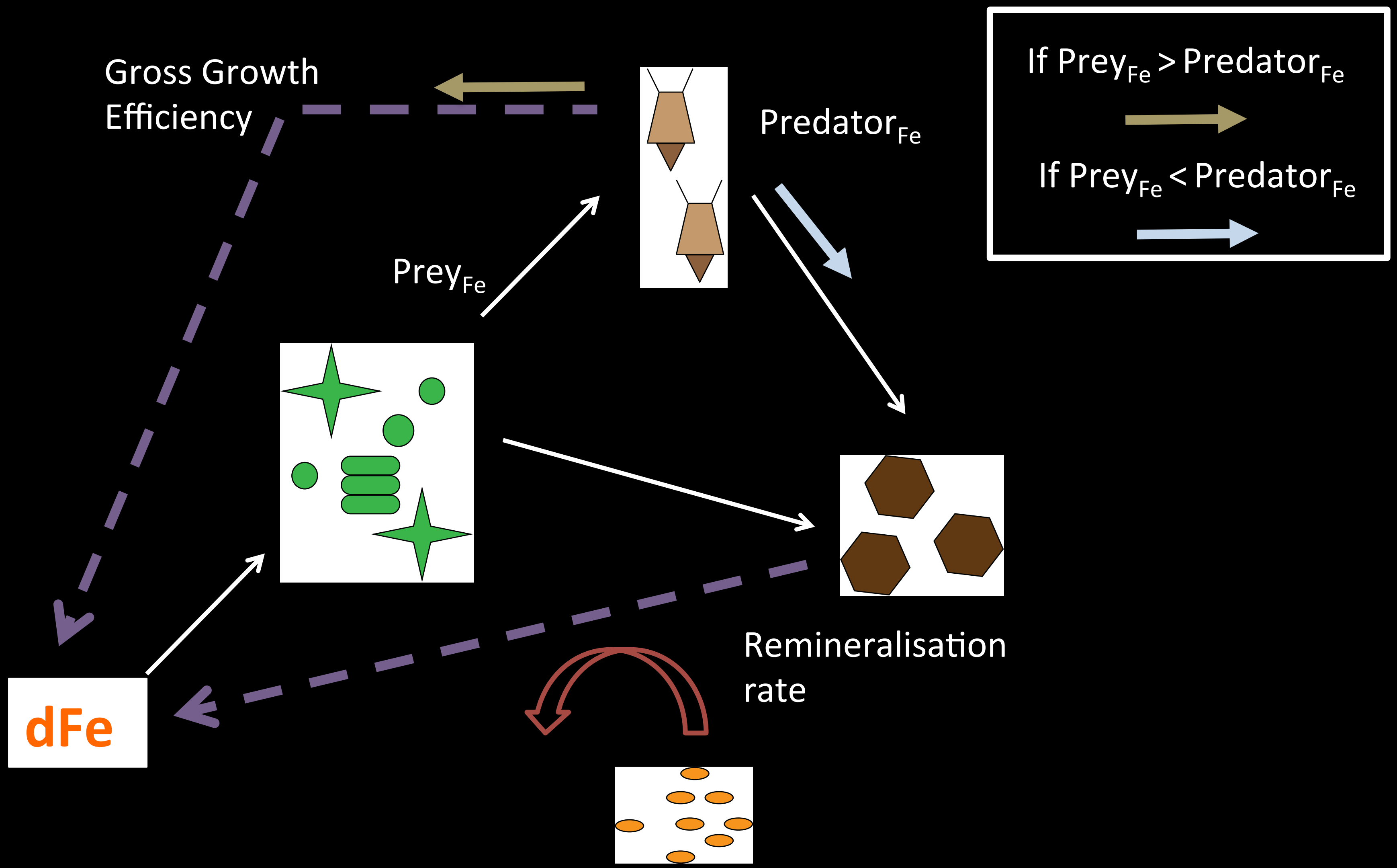


Recycling



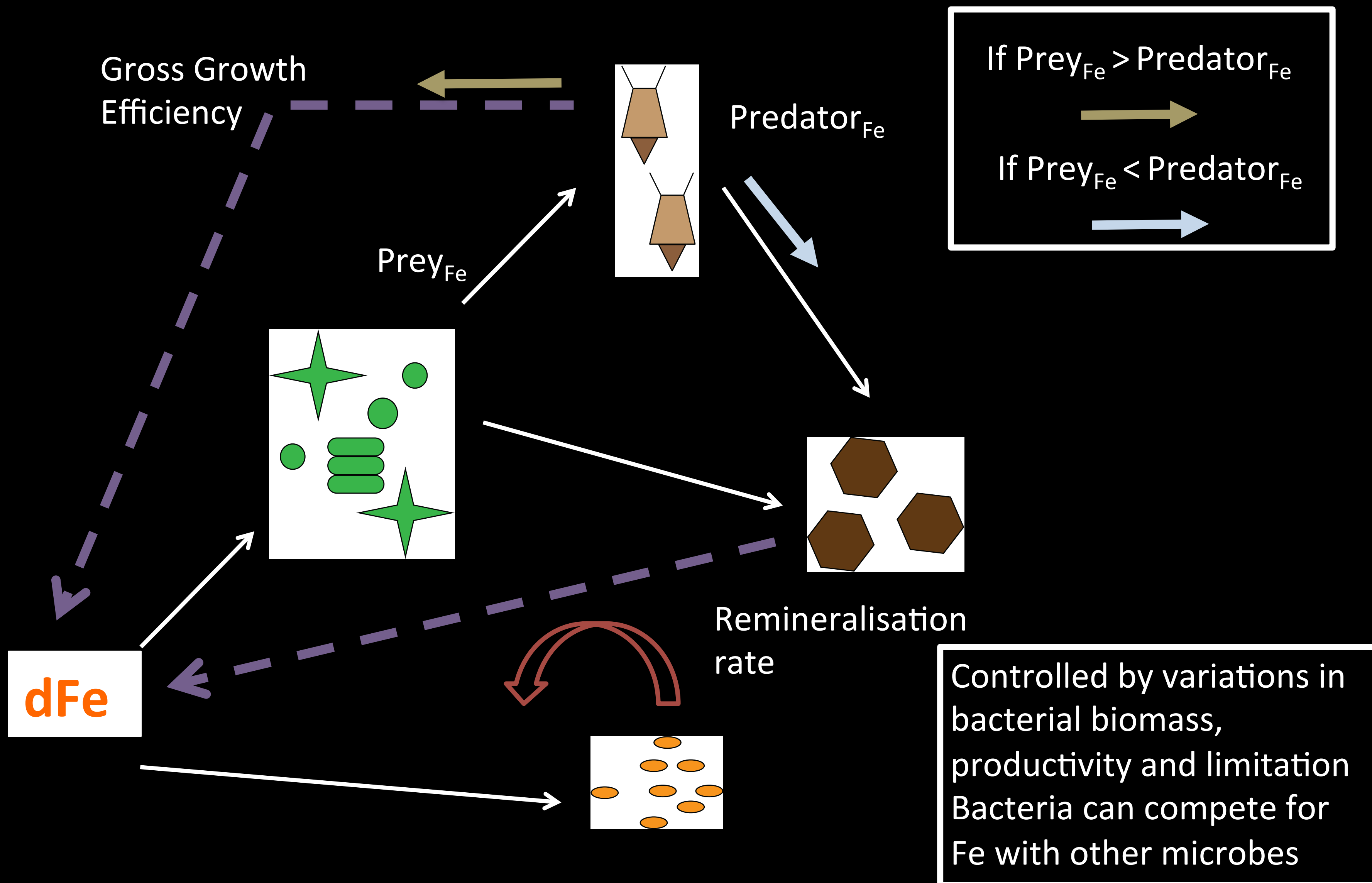
Often simply modelled
with fixed rates

Recycling



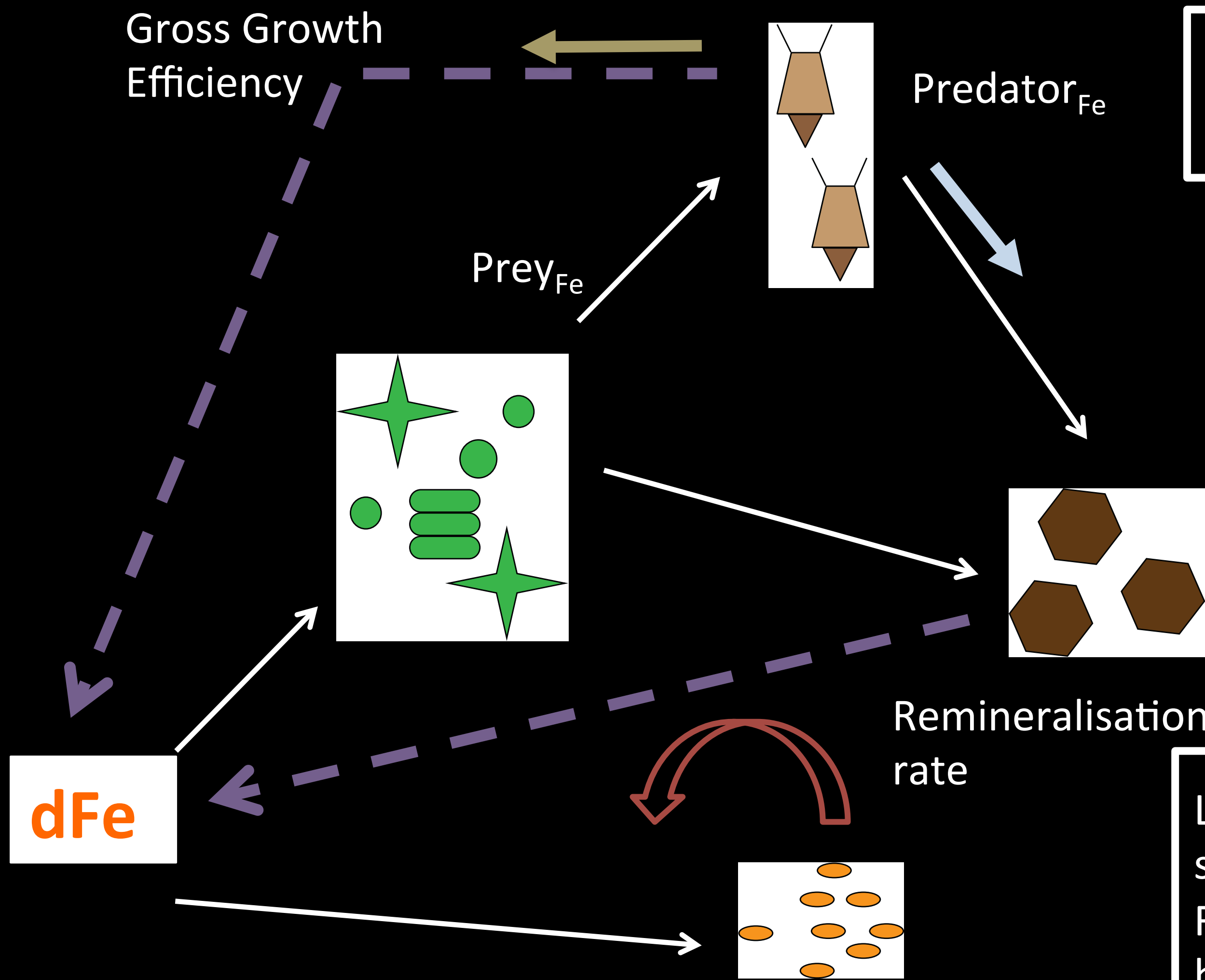
If $Prey_{Fe}$ > $Predator_{Fe}$
If $Prey_{Fe}$ < $Predator_{Fe}$
Gross Growth Efficiency
$Predator_{Fe}$
$Prey_{Fe}$
Remineralisation rate
dFe

Recycling



Gross Growth Efficiency
Predator$_{Fe}$
Prey$_{Fe}$
If Prey$_{Fe}$ > Predator$_{Fe}$
If Prey$_{Fe}$ < Predator$_{Fe}$
Remineralisation rate
dFe
Controlled by variations in bacterial biomass, productivity and limitation
Bacteria can compete for Fe with other microbes

Recycling – Key Parameters



GGE $Predator_{Fe}$

Lability and sinking speed of particulate Fe – how to model the bacteria?

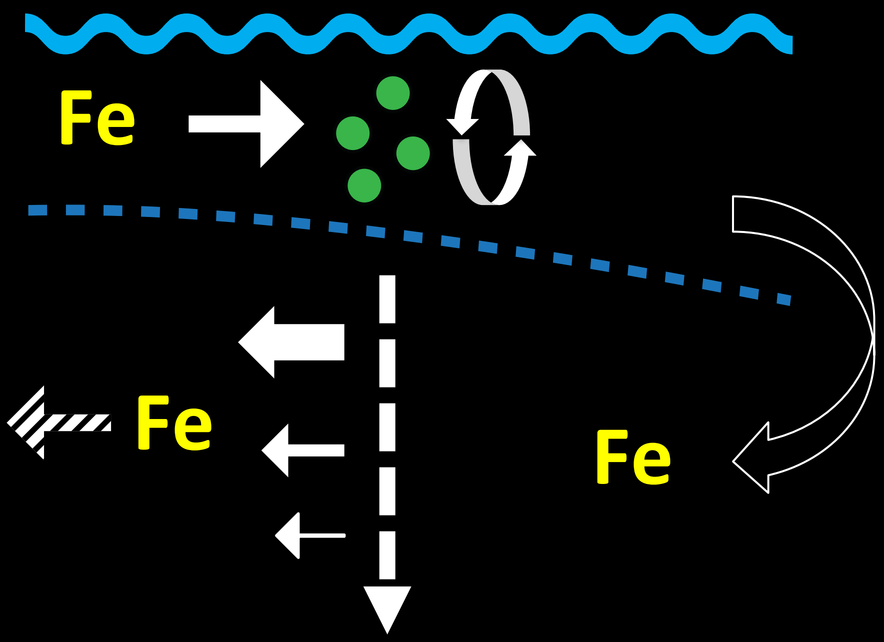
What are the main processes at play?

Surface uptake and cycling

~~Sinking and~~ regeneration

Scavenging

Subduction and transport



Scavenging

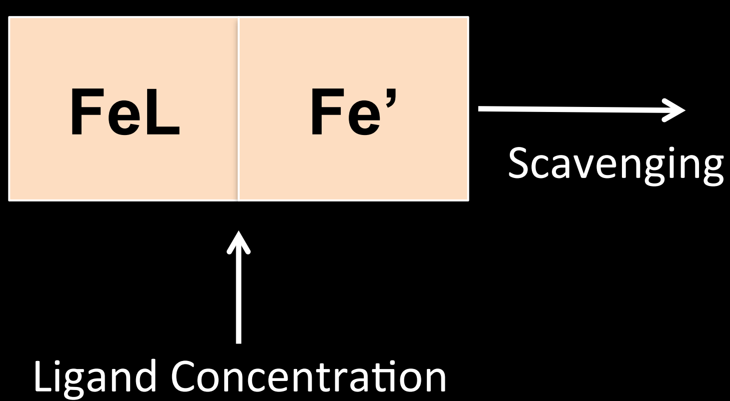
- Like other TEIs, iron is lost from the dissolved pool by ‘abiotic processes’
- Fundamental role for organic ligands

- Two main issues:
  - Speciation of Fe
  - ‘Loss’ of Fe from the dissolved pool

Speciation

- Key is to model how much Fe is complexed and how much is ‘free’

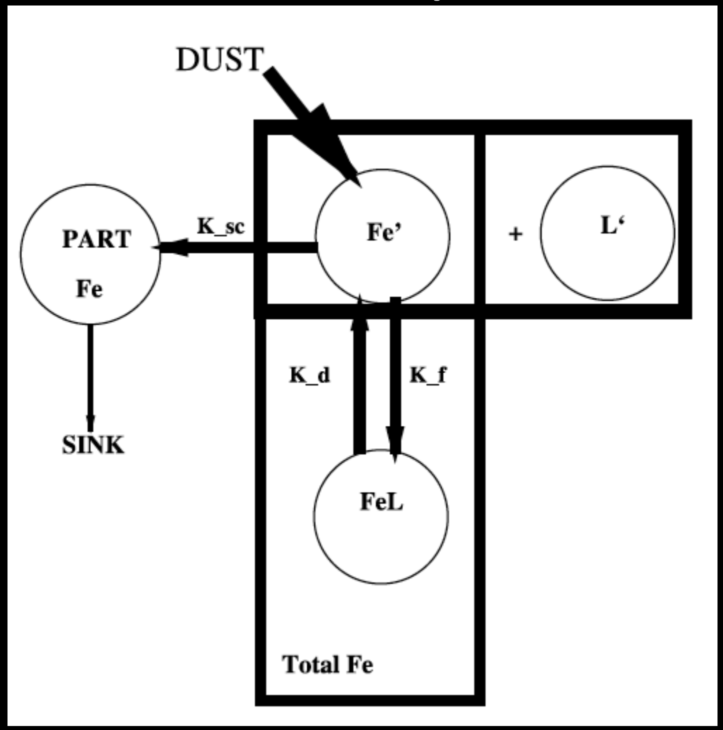
Threshold Model



Johnson et al. (1997, Mar Chem)

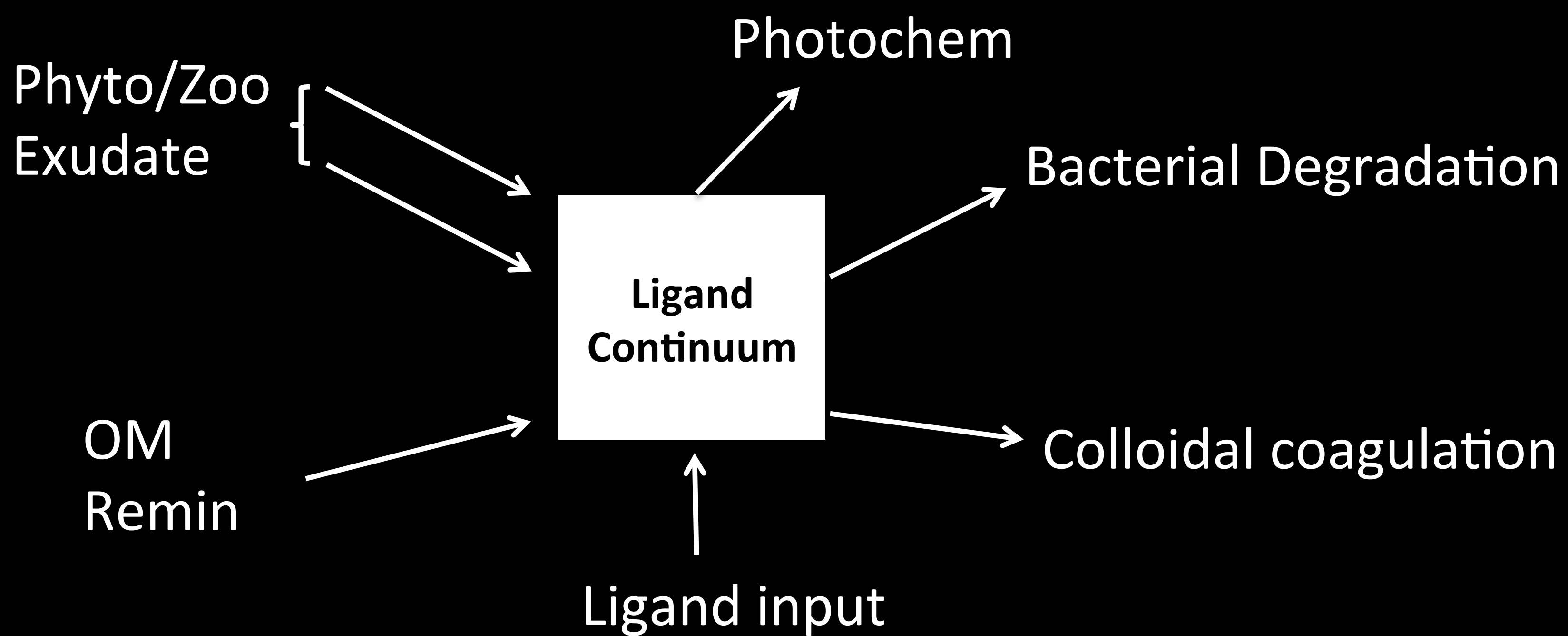
Requires information on [L] and K_{FeL}

Complexation Model



Parekh et al. (2004, GBC)

Dynamic Ligands



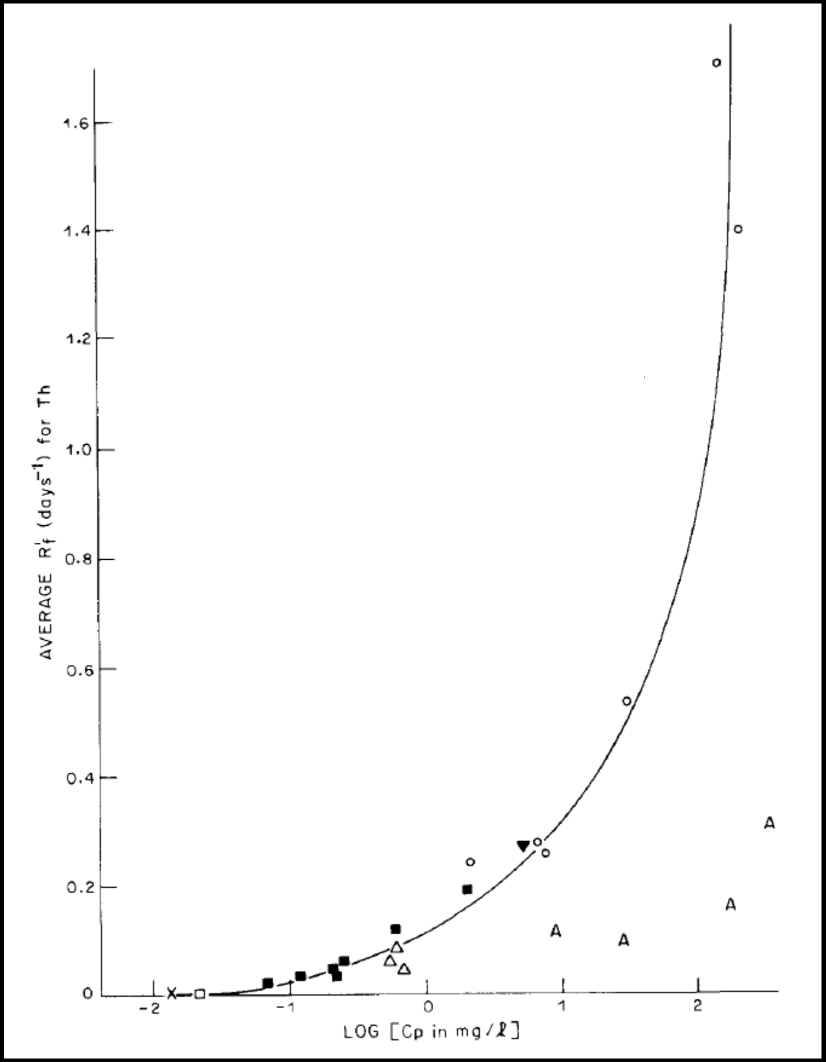
More attractive from a mechanistic standpoint, but requires more parameter choices (trade off)

Benchmarking these against other tracers (e.g. DOC production, O_2 consumption) is more helpful for models

Völker and Tagliabue (Mar Chem, 2015)

Loss from the dissolved pool

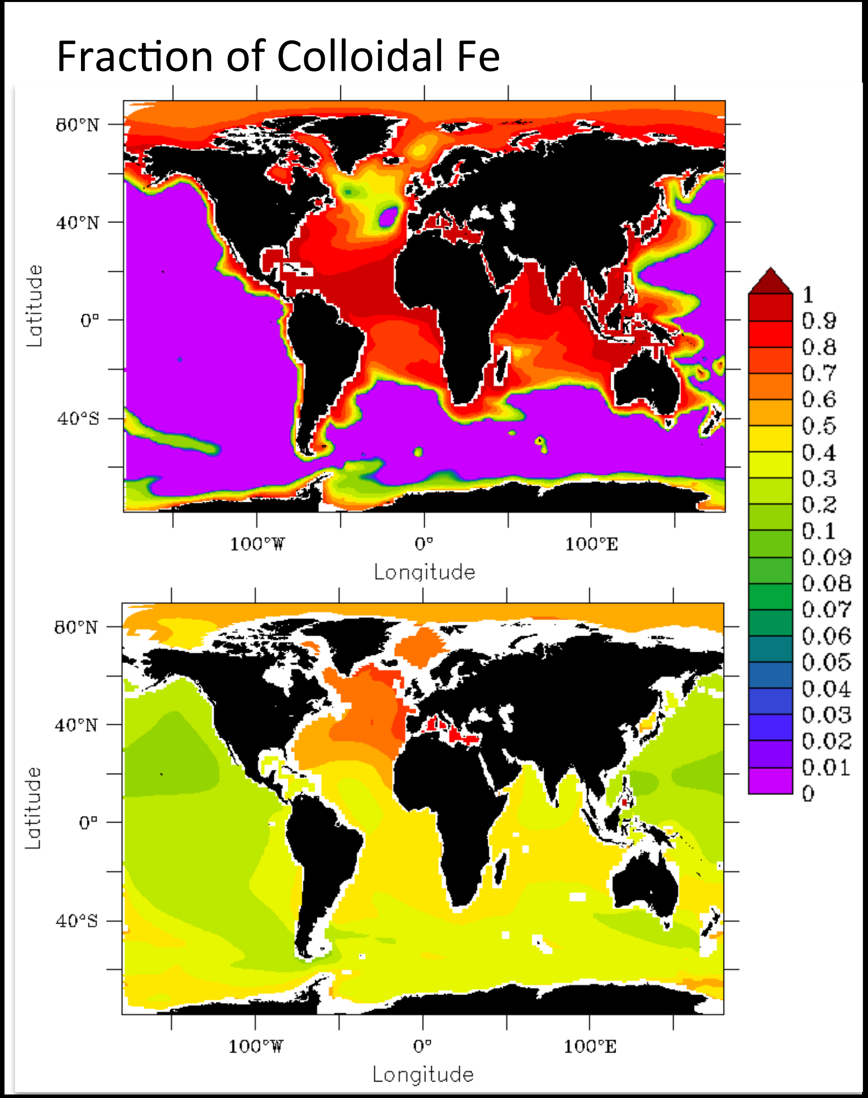
- Although a function of particle load, many models still use fixed rates
- At its most complex, scavenging is modelled as a function of particle load
- Crucial is the relative role played by each particle type (small and large POC, biogenic Si, calcite, lithogenics)
- Insights from other TEIs (e.g Pa/Th) potentially transformative



Honeyman et al (1988, DSR)

Colloidal Fe

- Important new datasets emerging on colloidal TEIs
- Usually ignored in models
- Where represented, relies on equilibrium speciation from laboratory studies
- Need to understand and represent unique roles for soluble and colloidal TEIs to further their representation in models



Tagliabue (unpub)

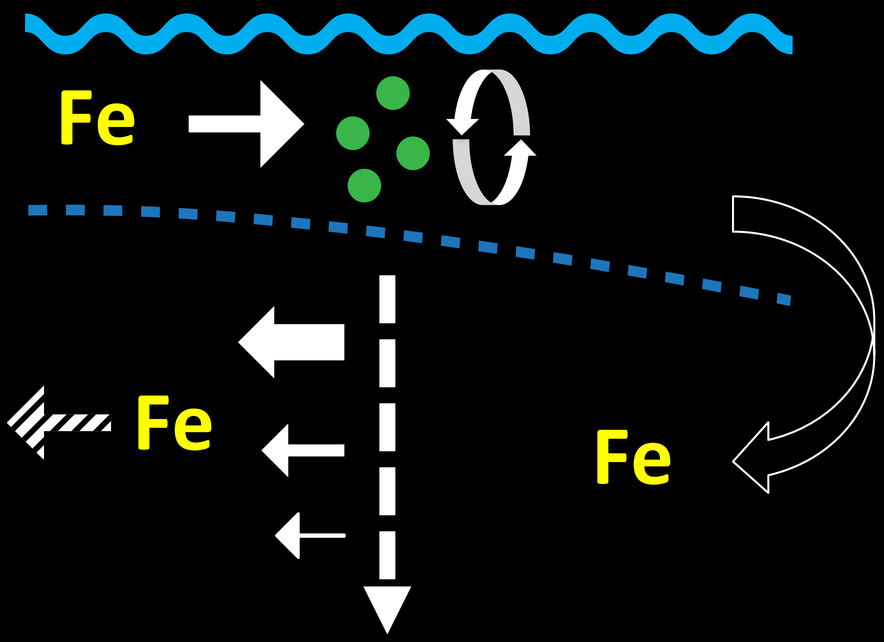
What are the main processes at play?

✓Surface uptake and cycling

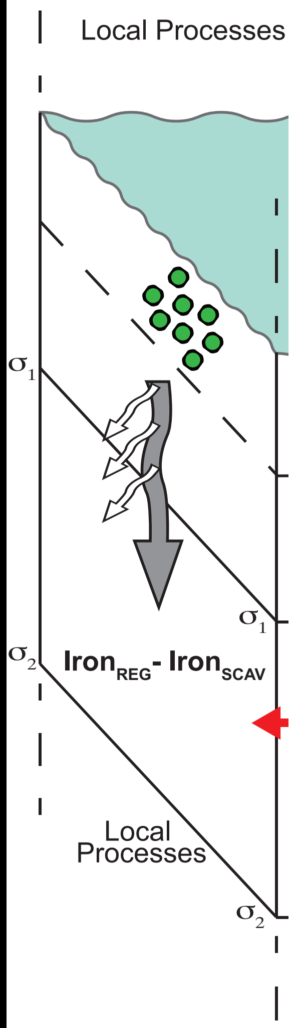
~~Sinking and~~ ✓regeneration

✓Scavenging

Subduction and transport



Subduction and Transport

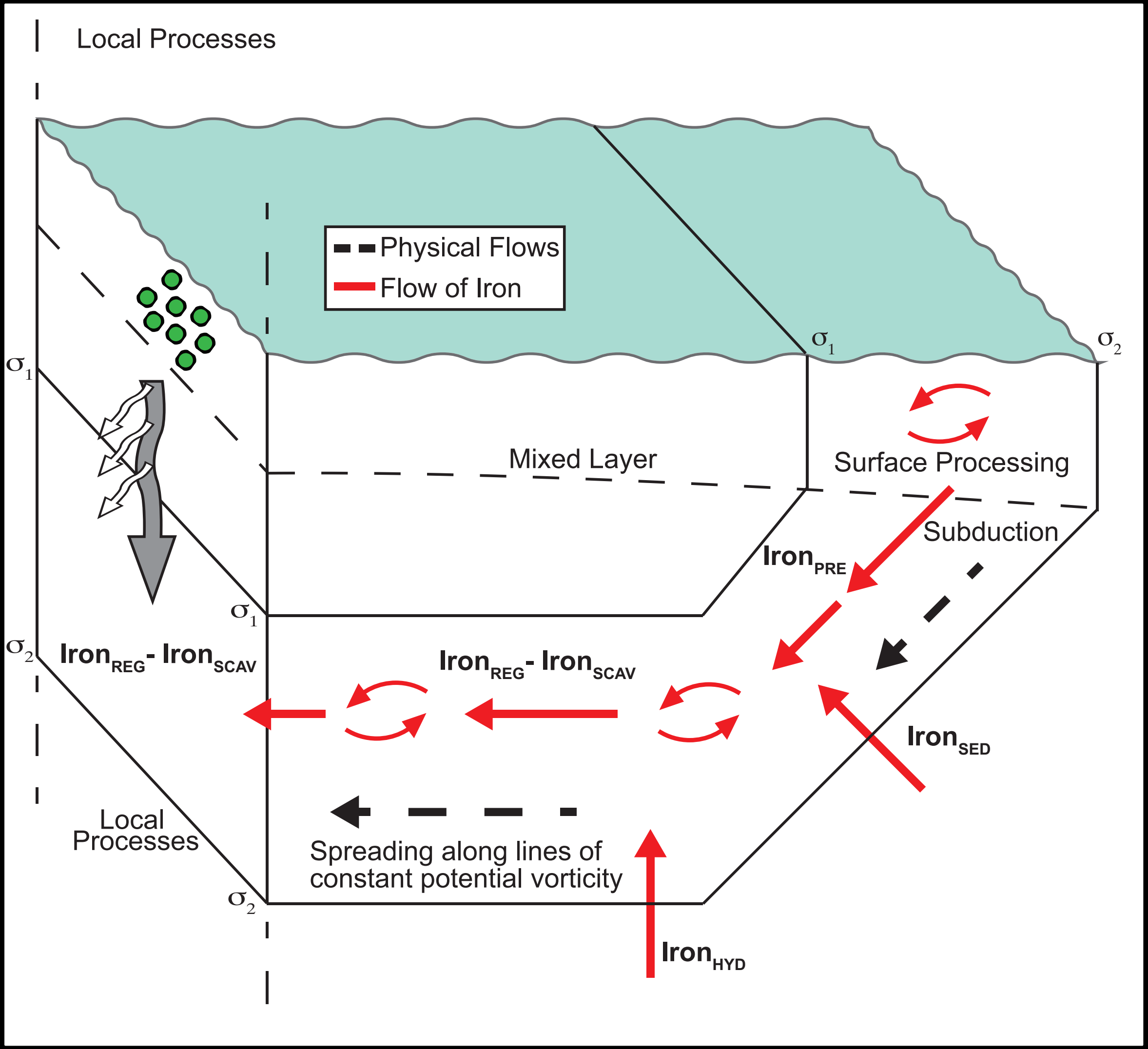


Observations made in one dimension need to be placed into their wider physical context

The interior concentration of any TEI has multiple components

$$DFe = DFe_{PRE} + DFe_{REG} + DFe_{SED} + DFe_{HYD} - DFe_{SCAV}$$

Subduction and Transport



$$DFe = DFe_{PRE} + DFe_{REG} + DFe_{SED} + DFe_{HYD} - DFe_{SCAV}$$

Summary of Processes and Assumptions

Surface uptake and cycling

- Affinity for Fe, quotas, physiology

Sinking and regeneration

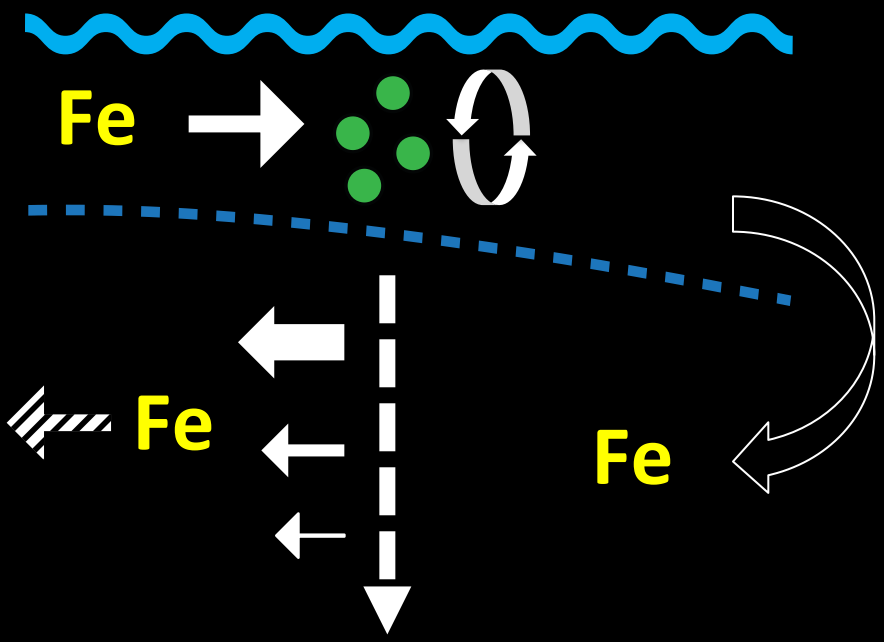
- TEI specific sinking or lability
- Zooplankton
- Bacteria

Scavenging

- Concentration and binding capacity of ligands
- 'Scavenging potential' of different particles

Subduction and transport

- Link physics to new theory / frameworks

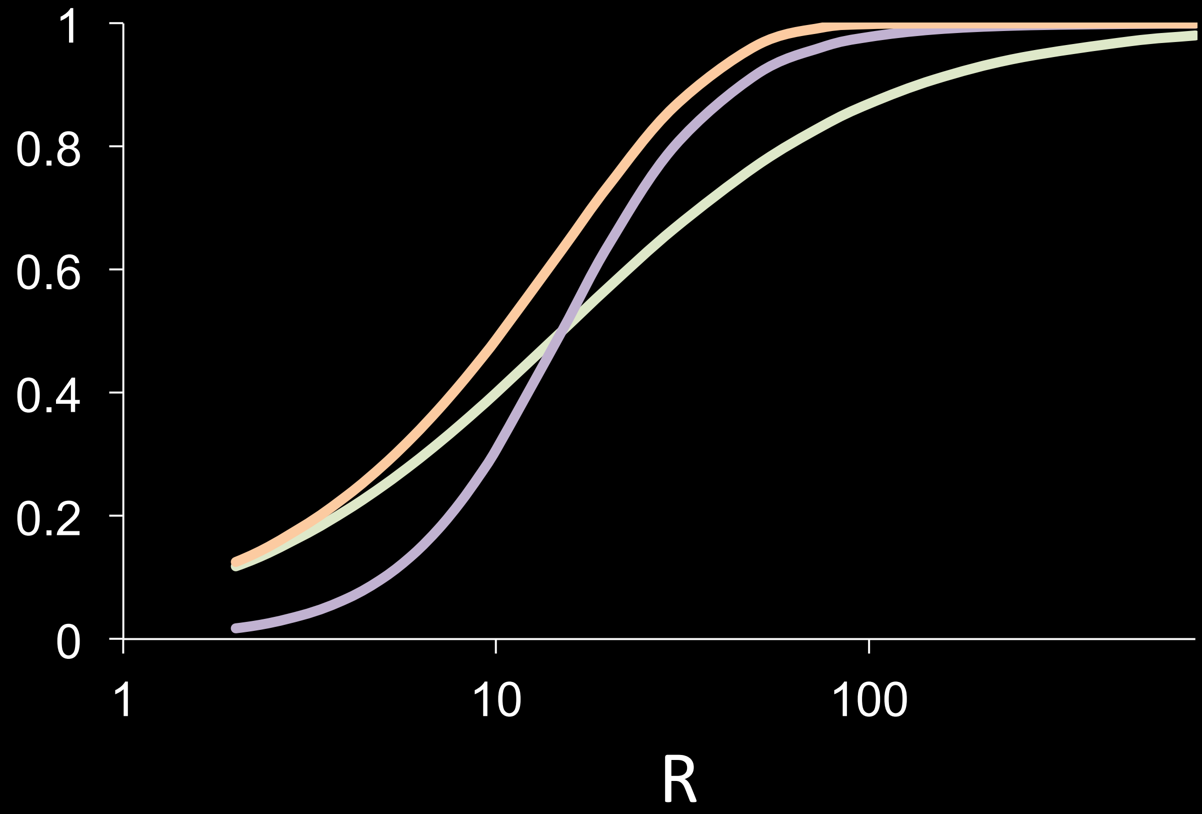


How are new processes added?

- Initially, fundamental mechanistic understanding is lacking
  - More approximate choices are needed!

How are new processes added?

- What are the underlying dependencies and the functional form?



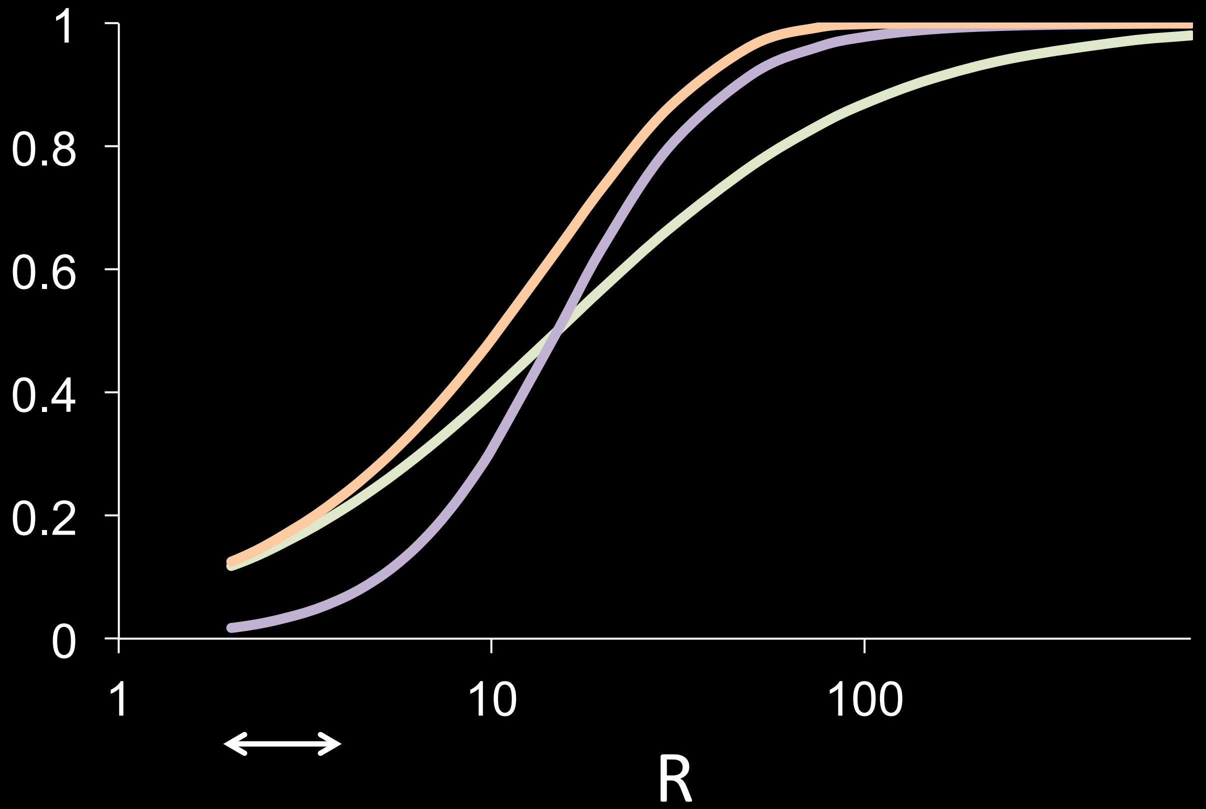
$$R/_{R+K_R}$$

$$R^2/_{R^2+K_R^2}$$

$$1-e^{R/_{K_R}}$$

How are new processes added?

- What are the underlying dependencies and the functional form?



$$R/_{R + K_R}$$

$$R^2/_{R^2 + K_R^2}$$

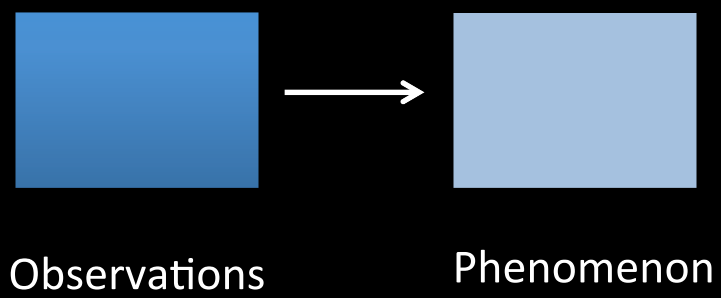
$$1 - e^{R/_{K_R}}$$

Thresholds can be imposed (e.g. oxygen based)

Where do we need to go?

- When built to represent key processes of interest, models can be fantastic hypothesis testing tools
  - Underpinned by their choice of parameterisations and parameters
- Close links between modellers and experimental scientists most fruitful
  - Lots of collaborative opportunity!
  - How can we exploit GEOTRACES section and process studies to identify and constrain the key processes so their wider relevance may be estimated?

How might we get there?

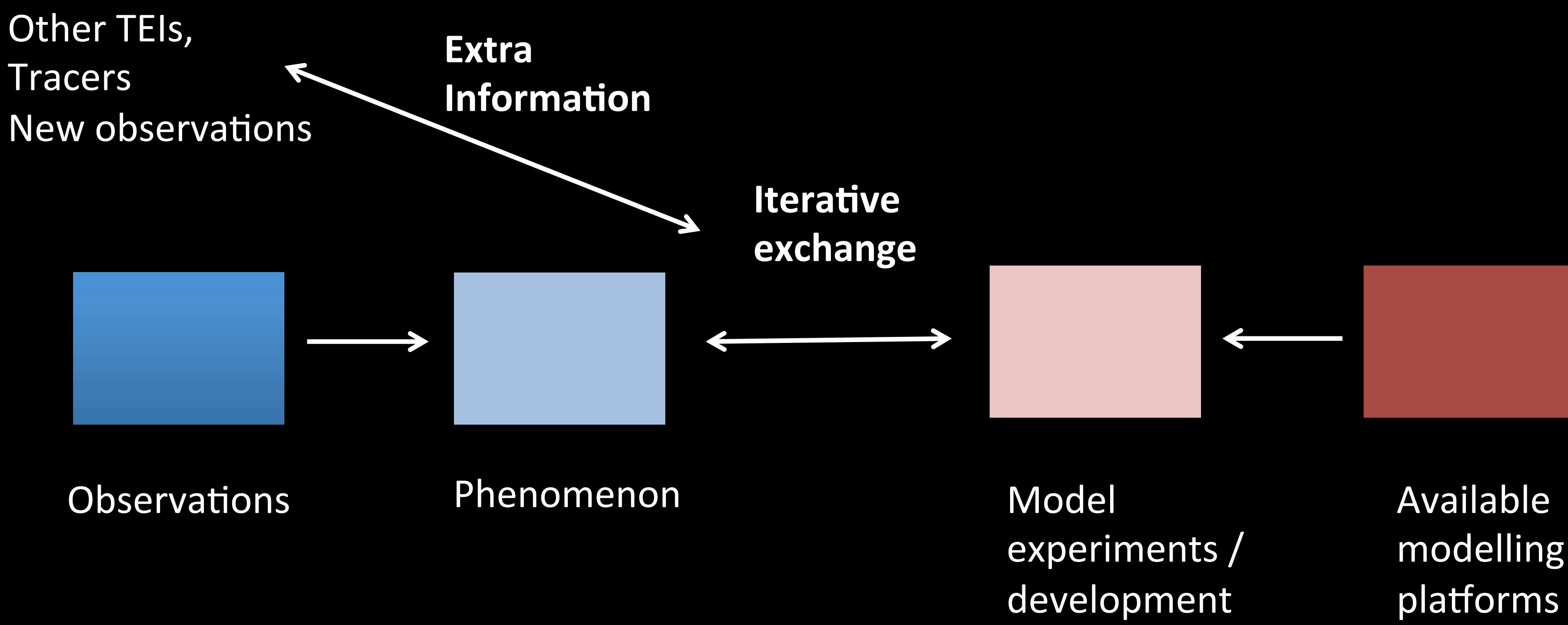


How important is this?

How might we get there?

How important is this?

How might we get there?



How important is this?

How might we get there?