**Concentration dependence of nitrogen isotope fractionation during ammonium assimilation by marine phytoplankton**

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**Model code**

dt = 0.0000333333333333 %hr

SAVE INTERVAL = 0.0005

{ INITIALIZATION EQUATIONS }

CellN14 = 1.66\*(1-0.00367)

CellN15 = 1.66\*0.00367

Gln14 = 0.005\*(1-0.00367)

Gln15 = 0.005\*0.00367

NH4cyt15 = 0.001\*0.00367

NH4cyt14 = 0.001\*(1-0.00367)

NH4out14 = 100\*(1-0.003695)

NH4out15 = 100\*0.003695

Vacuole14 = 1e-7\*(1-0.00367)

Vacuole15 = 1e-7\*(0.00367)

µmax = 0.8/24 %hr-1

VGSmax = µmax

alphaGS = 1.020

alphaCat = 1.005

MMLAU = NH4concOut/(30+NH4concOut)

MultLA = 0

MMHAU = NH4concOut/(0.05+NH4concOut)

MultHA = 8

PC\_NH3 = 1.8e-3\*60\*60

PC\_NH4 = 1.8e-6\*60\*60

BetaNH4 = 3.565

expBetaNH4 = 35.32

BetaVac = -0.396

expBetaVac = 0.673

SA = 5.3e-6

SAVac = 2.38e-6

Cell\_N\_total = CellN14+CellN15

"Cells\_L-1" = Cell\_N\_total/1.66e-6

CytoplasmNH4conc = (NH4cyt14+NH4cyt15)/("Cells\_L-1"\*1.15e-12)

CytoplasmNH3conc = CytoplasmNH4conc\*1e-7/1.76e-5 % at pH 7.0

NH4concOut = NH4out14+NH4out15

F15NH4out = NH4out15/(NH4out14+NH4out15)

NH3concOut = (NH4concOut)\*1.58e-6/1.76e-5 % at pH 8.2

Delta\_NH3in = (CytoplasmNH3conc-NH3concOut)

EffluxNH3 = PC\_NH3\*Delta\_NH3in\*SA/1000

d15NH4cyt = (((NH4cyt15/NH4cyt14)/0.00367)-1)\*1000

d15NH3cyt = d15NH4cyt-15

R15NH3cyt = (d15NH3cyt/1000+1)\*0.00367

F15NH3cyt = R15NH3cyt/(1+R15NH3cyt)

VENH314 = EffluxNH3\*"Cells\_L-1"\*(1-F15NH3cyt)

Delta\_NH4in = (CytoplasmNH4conc-NH4concOut\*expBetaNH4)/(1-expBetaNH4)

EffluxNH4 = -BetaNH4\*PC\_NH4\*Delta\_NH4in\*SA/1000

F15NH4cyt = NH4cyt15/(NH4cyt15+NH4cyt14)

VENH414 = EffluxNH4\*"Cells\_L-1"\*(1-F15NH4cyt)

VINH3Vac14 = 0\*InfluxNH3Vac\*"Cells\_L-1"\*(1-F15NH3cyt)

MMGS = CytoplasmNH4conc/(CytoplasmNH4conc+10)

GS14 = Cell\_N\_total\*VGSmax\*(1-F15NH4cyt)\*MMGS

GlnConc = (Gln14+Gln15)/("Cells\_L-1"\*1.15e-12)

MMGln = GlnConc/(GlnConc+700)

F15Gln = Gln15/(Gln14+Gln15)

Cat14 = 0.01\*Gln14

GOGAT14 = µmax\*Cell\_N\_total\*MMGln\*(1-F15Gln)

VENH315 = EffluxNH3\*"Cells\_L-1"\*F15NH3cyt

VENH415 = EffluxNH4\*"Cells\_L-1"\*F15NH4cyt

VINH3Vac15 = 0\*InfluxNH3Vac\*"Cells\_L-1"\*F15NH3cyt

GS15 = Cell\_N\_total\*VGSmax\*F15NH4cyt\*MMGS/alphaGS

Cat15 = 0.01\*Gln15/alphaCat

GOGAT15 = µmax\*Cell\_N\_total\*MMGln\*F15Gln

VENH4Vac14 = 0\*EffluxNH4Vac\*"Cells\_L-1"\*(1-F15NH4Vac)

VENH4Vac15 = 0\*EffluxNH4Vac\*"Cells\_L-1"\*F15NH4Vac

VU14 = (MMLAU\*MultLA+MMHAU\*MultHA)\*µmax\*Cell\_N\_total\*(1-F15NH4out)

alphaTR = 0\*(25/(1+EXP((30-NH4concOut)/2)))/1000+1

VU15 = ((MultLA\*MMLAU\*µmax\*F15NH4out\*Cell\_N\_total)+(MultHA\*MMHAU\*µmax\*F15NH4out\*Cell\_N\_total))/alphaTR

d15NCell = (((CellN15/CellN14)/0.00367)-1)\*1000

d15NH4Vac = (((Vacuole15/Vacuole14)/0.00367)-1)\*1000

d15NH3Vac = d15NH4Vac-15

d15NH4out = (((NH4out15/NH4out14)/0.00367)-1)\*1000

NH4concVac = (Vacuole14+Vacuole15)/("Cells\_L-1"\*3.45e-13)

NH3concVac = NH4concVac\*1e-9/1.76e-5 % at pH 5.0

Delta\_NH3Vac = (CytoplasmNH3conc-NH3concVac)

Delta\_NH4Vac = (NH4concVac-CytoplasmNH4conc\*expBetaVac)/(1-expBetaVac)

EffluxNH4Vac = -BetaVac\*PC\_NH4\*Delta\_NH4Vac\*SAVac/1000

F15NH4Vac = Vacuole15/(Vacuole14+Vacuole15)

InfluxNH3Vac = PC\_NH3\*Delta\_NH3Vac\*SAVac/1000

{ RUNTIME EQUATIONS }

CellN14(t) = CellN14(t - dt) + (GOGAT14) \* dt {NON-NEGATIVE}

CellN15(t) = CellN15(t - dt) + (GOGAT15) \* dt {NON-NEGATIVE}

Gln14(t) = Gln14(t - dt) + (GS14 - Cat14 - GOGAT14) \* dt {NON-NEGATIVE}

Gln15(t) = Gln15(t - dt) + (GS15 - Cat15 - GOGAT15) \* dt {NON-NEGATIVE}

NH4cyt15(t) = NH4cyt15(t - dt) + (VU15 + VENH4Vac15 + Cat15 - VENH315 - VENH415 - VINH3Vac15 - GS15) \* dt {NON-NEGATIVE}

NH4cyt14(t) = NH4cyt14(t - dt) + (VU14 + VENH4Vac14 + Cat14 - VENH314 - VENH414 - VINH3Vac14 - GS14) \* dt {NON-NEGATIVE}

NH4out14(t) = NH4out14(t - dt) + (VENH314 + VENH414 - VU14) \* dt {NON-NEGATIVE}

NH4out15(t) = NH4out15(t - dt) + (VENH315 + VENH415 - VU15) \* dt {NON-NEGATIVE}

Vacuole14(t) = Vacuole14(t - dt) + (VINH3Vac14 - VENH4Vac14) \* dt {NON-NEGATIVE}

Vacuole15(t) = Vacuole15(t - dt) + (VINH3Vac15 - VENH4Vac15) \* dt {NON-NEGATIVE}