

SOLUTION_MASTER_SPECIES
 N(-3) NH4+ 0.0 N
 SOLUTION_SPECIES
 NH4+ = NH3 + H+
 log_k -9.252
 delta_h 12.48 kcal
 -analytic 0.6322 -0.001225 -2835.76

NO3- + 10 H+ + 8 e- = NH4+ + 3 H2O
 log_k 119.077
 delta_h -187.055 kcal
 -gamma 2.5000 0.0000

SOLUTION 1 LAKE MEDARD MONIMOLIMNION'S WATER (quite imbalanced)

units	ppm	# unless otherwise stated
pH	7.6	
density	1.002	
temp	8.0	
pe	-3	
Ca	6.09	
Mg	15.01	
Na	163591	ppb
K	8004	ppb
Al	0.0027	
Mn	1.78	pe
Si	5274	ppb
Cl	192073	ppb
S(6)	1575.4	
S(-2)	4.263	ppb # L.Q. AVS
N(5)	1.116	ppm as NO3
N(-3)	2.345	ppm as NH4
Fe	1.83	pe
C(4)	397	

END

EQUILIBRIUM_PHASES 1

Calcite	0.0	CO2(g)	1	# Add CO2(g) until calcite saturation
FIX_H+	-7.6	NaOH	10	# Add NaOH to pH 7.6
Halite	-3.7	10		# Optimze conduct. to environmentally relevant values.
Dolomite	-1.87	0		

PHASES
 # Auxiliar phase used to fix pH
 FIX_H+
 H+ = H+
 logK 0

END
 TITLE pH is adjusted to measured monimolimic values; conductance and pe OK,
 environemntally relevant [C(4)] levels obtained by iteration of dolomite SI: error
 significantly optimized
 USE solution 1
 USE equilibrium_phases 1
 END