set all oxidation of H2S to SO4 or CH4 to SO4 at boundaries to zero: % no secondary redox!

**MATLAB**:

SO4: FH2S to zox line **106**; FSO4 at zso4 line **181**

H2S: zso4FH2S at zso4 line **53**; zoxFH2S at zox line **79**

O2: FO2 at zox line **133**

ALK: zso4FALK line **71**, zoxFALK line **97**

**FORTRAN**:

in initialize: NC1, NC2, ALKRNIT, ALKRH2S, ALKRMET, ALKRAOM

O2: FUN\_huelseetal2016\_calcFO2 lines **1433**

SO4: FH2S to zox lines **1853**; FUN\_calcFSO4 to zso4 lines **1962**

H2S: zso4FH2S to zso4 line **2233**; zoxFH2S to zox line **2271**

ALK: zso4FALK: line **2836**, zoxFALK: **2865**

--> should get mass conservation of SO4 + H2S, also check how ALK changed

**PRE-INDUSTRIAL SETUP**

**############# 21.03.2017**

USE base-config WITH 8 OCEAN-LEVELS: cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES.config

WITHOUT Fe

GENERAL SETUP: as befre with artificial world

user-config generally: no gas-transfer, no weathering, no CaCO3 burial → test conservation of mass

OMEN-SED: here now, no secondary redox! - all remineralised

0) Biotic, No OMEN-SED

job 9804

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_00\_worbe2.S36x36\_nogas\_noweather\_open\_NoOMEN 10000

1) k = 0.01

job 9805

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_01\_worbe2.S36x36\_nogas\_noweather\_open\_k\_0.01 10000

2) k = 0.05

job 9806

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_02\_worbe2.S36x36\_nogas\_noweather\_open\_k\_0.05 10000

3) k = 0.1

job 9807

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_03\_worbe2.S36x36\_nogas\_noweather\_open\_k\_0.1 10000

4) k = 1.0

job 9808

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_04\_worbe2.S36x36\_nogas\_noweather\_open\_k\_1.0 10000

5) k = 4.0

job 9809

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_05\_worbe2.S36x36\_nogas\_noweather\_open\_k\_4.0 10000

**-----------------------------------------------------------------------------**

**NOW with 16 ocean levels**

**-----------------------------------------------------------------------------**

base-config: **cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES.config**

0) Biotic, No OMEN-SED

job 9812

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_00\_worjh2\_nogas\_noweather\_open\_NoOMEN 10000

1) k = 0.01 -----> **499.5 years netcdf error: NetCDF: Numeric conversion not representable**

**trace string: putvar2d fsedocn\_O2**

job 9813

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_01\_worjh2\_nogas\_noweather\_open\_k\_0.01 10000

2) k = 0.05

job 9814

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_02\_worjh2\_nogas\_noweather\_open\_k\_0.05 10000

3) k = 0.1

job 9815

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_03\_worjh2\_nogas\_noweather\_open\_k\_0.1 10000

4) k = 1.0

job 9816

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_04\_worjh2\_nogas\_noweather\_open\_k\_1.0 10000

5) k = 4.0

job 9817

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_05\_worjh2\_nogas\_noweather\_open\_k\_4.0 10000

**############# 22.03.2017**

--------- **RUN ocean 16 level** with k = 0.01 for 495 years because crashed after 499.5 years (see yesterday run 1) )

6) k = 0.01

(problem was: 499.5 years netcdf error: NetCDF: Numeric conversion not representable; trace string: putvar2d fsedocn\_O2)

job 9839

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2203\_06\_worjh2\_nogas\_noweather\_open\_k\_0.01\_495years 495

**--------- RUN YESTERDAY 8 ocean level runs for 20,000 years as not in equilibrium**

0) Biotic, No OMEN-SED

job 9840

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2203\_00\_worbe2.S36x36\_nogas\_noweather\_open\_NoOMEN\_20kyrs 20000

1) k = 0.01

job 9841

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2203\_01\_worbe2.S36x36\_nogas\_noweather\_open\_k\_0.01\_20kyrs 20000

2) k = 0.05

job 9842

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2203\_02\_worbe2.S36x36\_nogas\_noweather\_open\_k\_0.05\_20kyrs 20000

3) k = 0.1

job 9843

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2203\_03\_worbe2.S36x36\_nogas\_noweather\_open\_k\_0.1\_20kyrs 20000

4) k = 1.0

job 9844

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2203\_04\_worbe2.S36x36\_nogas\_noweather\_open\_k\_1.0\_20kyrs 20000

5) k = 4.0

job 9845

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worbe2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2203\_05\_worbe2.S36x36\_nogas\_noweather\_open\_k\_4.0\_20kyrs 20000

**############# 27.03.2017**

--------- **RUN ocean 16 level** with k = 0.01 for 490 years because very postive BW concentrations already after 495 years establised (see 22.03. run 6) )

(problem was: 499.5 years netcdf error: NetCDF: Numeric conversion not representable; trace string: putvar2d fsedocn\_O2)

1) k = 0.01

job 10036

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2703\_01\_worjh2\_nogas\_noweather\_open\_k\_0.01\_490years 490

2) as 1) k = 0.01 run for 480 years, in case O2 already weird at 490 years

job 10037

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2703\_02\_worjh2\_nogas\_noweather\_open\_k\_0.01\_480years 480

3) k = 0.01 – now check for bottom water [O2] > 1 microM (or micro mol kg-1) = 1E-9 mol/cm^3

job 10038

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2703\_03\_worjh2\_nogas\_noweather\_open\_k\_0.01\_O2\_1E-9 10000

4) k = 0.01 – now check for bottom water [O2] > 10 microM (or micro mol kg-1) = 10E-9 mol/cm^3

job 10039

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2703\_04\_worjh2\_nogas\_noweather\_open\_k\_0.01\_O2\_10E-9 10000

**----------- 16 ocean level setup: now set minimum sedimentationrate to 5.0e-4 instead of 4.0e-4 …. check if k=0.01 is not crashing anymore and if results look OK**

1) k = 0.01

job 10041

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2703\_01\_worjh2\_nogas\_noweather\_open\_k\_0.01\_w\_5e-4 10000

2) k = 0.05

job 10042

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2703\_02\_worjh2\_nogas\_noweather\_open\_k\_0.05\_w\_5e-4 10000

3) k = 0.1

job 10043

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2703\_03\_worjh2\_nogas\_noweather\_open\_k\_0.1\_w\_5e-4 10000

4) k = 1.0

job 10044

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2703\_04\_worjh2\_nogas\_noweather\_open\_k\_1.0\_w\_5e-4 10000

5) k = 4.0

job 10045

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg.worjh2.BASES DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2703\_05\_worjh2\_nogas\_noweather\_open\_k\_4.0\_w\_5e-4 10000

**----------- artifical ocean using the complete OMEN model**

**no air-sea gas, no weathering, no CaCO3 burial**

**using simple Ocean setup with shelves: cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES**

**…. check how results look like now (especially ALK) as now with secondary redox reactions**

**[O2] increases, [H2] decreases... 6\_EXP\_Shelves\_2703\_TOTAL\_Full\_OMEN.eps**

**apparently not all H2S is oxidized, maybe problem with zoxgf as this has a big impact for very small zox...**

6) k=0.01

job 10046

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2703\_06\_shelves\_nogasweath\_k\_0.01\_OMEN\_ALL 10000

7) k=0.05

job 10047

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2703\_07\_shelves\_nogasweath\_k\_0.05\_OMEN\_ALL 10000

8) k=0.1

job 10048

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2703\_08\_shelves\_nogasweath\_k\_0.1\_OMEN\_ALL 10000

9) k=1.0

job 10049

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2703\_09\_shelves\_nogasweath\_k\_1.0\_OMEN\_ALL 10000

10) k=4.0

job 10050

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2703\_10\_shelves\_nogasweath\_k\_4.0\_OMEN\_ALL 10000

**############# 28.03.2017**

**----------- artifical ocean using the complete OMEN model, no air-sea gas, no weathering, no CaCO3 burial**

**using simple Ocean setup with shelves: cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES**

**…. now with zoxgf = 0.0 (compare results yesterday)**

**---> no significant change in results! 6\_EXP\_Shelves\_2803\_TOTAL\_Full\_OMEN\_zoxgf\_0.eps**

1) k=0.01

job 10060

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_01\_shelves\_nogasweath\_k\_0.01\_OMEN\_ALL 10000

2) k=0.05

job 10061

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_02\_shelves\_nogasweath\_k\_0.05\_OMEN\_ALL 10000

3) k=0.1

job 10062

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_03\_shelves\_nogasweath\_k\_0.1\_OMEN\_ALL 10000

4) k=1.0

job 10063

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_04\_shelves\_nogasweath\_k\_1.0\_OMEN\_ALL 10000

**---------- same as 1) – 4) but now set conzinf = 0.0 if it is < 0.0, otherwise advextive flux wrong... zoxgf = 0.1**

**---> no significant change in results! 5\_EXP\_Shelves\_2803\_TOTAL\_Full\_OMEN\_zoxgf\_01\_conczinf\_0.eps**

5) k=0.01

job 10064

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_05\_shelves\_nogasweath\_k\_0.01\_OMEN\_ALL 10000

6) k=0.05

job 10065

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_06\_shelves\_nogasweath\_k\_0.05\_OMEN\_ALL 10000

7) k=0.1

job 10066

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_07\_shelves\_nogasweath\_k\_0.1\_OMEN\_ALL 10000

**--------- same as 1) – 4) set conzinf = 0.0 if it is < 0.0, zoxgf = 0.1**

**here change stoichiometry for H2S oxidation to O2H2S = 2.0 (was 1.0) …. should use more OS now with 2nd redox**

8) k=0.01

job 10068

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_08\_shelves\_nogasweath\_k\_0.01\_OMEN\_ALL\_newO2H2S 10000

9) k=0.05

job 10069

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_09\_shelves\_nogasweath\_k\_0.05\_OMEN\_ALL\_newO2H2S 10000

10) k=0.1

job 10070

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_10\_shelves\_nogasweath\_k\_0.1\_OMEN\_ALL\_newO2H2S 10000

11) k=1.0

job 10071

qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh cgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.\_rwlma.BASES DOM/08\_OMEN\_GENIE\_March2017 2803\_11\_shelves\_nogasweath\_k\_1.0\_OMEN\_ALL\_newO2H2S 10000

*---------------------------------------------------------------------------*

*Next one use maybe, this includes GEMLITE, can I just say false to switch it off?*

*-----------------------------------------------------------------------------*

*NOW with FE and 16 ocean levels (but DOM: without GEMLITE):*

*base-config:* ***DOMcgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.worjh2.BASESFe.config***

*0) Biotic, No OMEN-SED*

*job*

*qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh DOMcgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.worjh2.BASESFe DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_00\_worjh2.S36x36\_nogas\_noweather\_open\_NoOMEN\_Fe 10000*

*1) k = 0.01*

*job*

*qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh DOMcgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.worjh2.BASESFe DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_01\_worjh2.S36x36\_nogas\_noweather\_open\_k\_0.01\_Fe 10000*

*2) k = 0.05*

*job*

*qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh DOMcgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.worjh2.BASESFe DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_02\_worjh2.S36x36\_nogas\_noweather\_open\_k\_0.05\_Fe 10000*

*3) k = 0.1*

*job*

*qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh DOMcgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.worjh2.BASESFe DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_03\_worjh2.S36x36\_nogas\_noweather\_open\_k\_0.1\_Fe 10000*

*4) k = 1.0*

*job*

*qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh DOMcgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.worjh2.BASESFe DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_04\_worjh2.S36x36\_nogas\_noweather\_open\_k\_1.0\_Fe 10000*

*5) k = 4.0*

*job*

*qsub -j y -o cgenie\_output -V -S /bin/bash runmuffin.sh DOMcgenie.eb\_go\_gs\_ac\_bg\_sg\_rg\_gl.worjh2.BASESFe DOM/09\_OMEN\_GENIE\_PreInd\_March2017 2103\_05\_worjh2.S36x36\_nogas\_noweather\_open\_k\_4.0\_Fe 10000*