// reactions //

/\* SI \*/ reac1 = 0.0;

/\* SS \*/ reac2 =

/\* XI \*/ reac3 = 0.0;

/\* XS \*/ reac4 =

/\* XBH \*/ reac5 =

/\* XBA1 \*/ reac6 =

/\* XU \*/ reac7 =

/\* SO2 \*/ reac8 = ((-(2.2857143 / (Y\_A1\*n\_Y\_AOB)) - 1.0))\*proc10;

/\* SNO3 \*/ reac9 =

/\* SNH \*/ reac10 = ( - (1.0 / (Y\_A1\*n\_Y\_AOB)) - i\_X\_B)\*proc9 +

/\* SND \*/ reac11 =

/\* XND \*/ reac12 =

/\* SALK \*/ reac13 = ( - i\_X\_B / 14.0) - (1.0 / (7.0 \* (Y\_A1\*n\_Y\_AOB)))\*proc10;

/\* SNO2 \*/reac16 =

/\* SNO \*/reac17 =

/\* SN2O \*/reac18 =

/\* SN2 \*/reac19 =

/\* XBA2 \*/reac20 =

proc1 =

proc2x1 =

proc2x2 =

proc2x3 =

proc2x4 =

proc3x1 =

proc3x2 =

proc4 =

proc5x1 =

proc5x2 =

proc6 =

proc7 =

proc8 =

proc9 =

proc10 = + S\_FA)) \* (xtemp[7]/(K\_SO\_AOBden2 + (1-2\*pow((K\_SO\_AOBden2/K\_IO\_AOBden2),0.5)) \* xtemp[7] + (pow(xtemp[7],2.0)/K\_IO\_AOBden2))));

KLa\_temp =

Kla\_N2O =

Kla\_NO =

Kla\_N2 =

Flux\_NO =

Flux\_N2O =

Flux\_N2 =

// calculation of free ammonia

KB\_2\_KW =

S\_FA =

// calculation of free nitrous acid //

K\_A =

S\_FNA =

/\* temperature compensation \*/

mu\_H\_Temp =

mu\_A1\_Temp =

mu\_A2\_Temp =

b\_H\_Temp =

b\_A1\_Temp =

b\_A2\_Temp =

k\_h\_Temp =

k\_a\_Temp =

SO\_sat\_temp = 0.9997743214\* (8.0/ 10.5\*( 56.12\* 6791.5\* exp(- 66.7354 + 87.4755/(( x[15]+ 273.15)/ 100.0) + 24.4526\* log((x[15]+273.15)/ 100.0)))); /\* van't Hoff equation \*/

KLa\_temp =

// calculation of free ammonia

KB\_2\_KW = exp(6344.0/(273.15 + x[15]));

S\_FA = (x[9]\*pow(10,pH))/(KB\_2\_KW + pow(10,pH));

// calculation of free nitrous acid //

K\_A = exp(-2300.0/(273.15+ x[15]));

S\_FNA = (x[16] \* 1.0 / (1.0 + K\_A \* pow(10,pH)));

// calculation of the total oxidazed nitrogen

S\_NOX =

// specific KLa //

Kla\_N2O = pow(D\_N2O,0.5) / pow(D\_O2,0.5) \* KLa\_temp;

Kla\_NO = pow(D\_NO,0.5) / pow(D\_N2O,0.5) \* Kla\_N2O;

Kla\_N2 = pow(D\_N2,0.5) / pow(D\_N2O,0.5) \* Kla\_N2O;

y[13] = // XTSS