OLI Software 12.0
Databank Updates

March 18, 2024

Mixed-solvent electrolyte (MSE) thermophysical property databanks

Complexes between Fe and organic species

Fe (II, III) – acetate
Fe (II, III) – diethylenetriamine
Fe (II, III) – ethylenediamine
Fe (II, III) – glycine
Fe (II, III) – pyrozole
Fe (II, III) – catechol
Fe (II, III) – gallic acid
Fe (II, III) – humic acid
Fe (II, III) – phenol

Butyric acid revision, including Ca and K butyrate and butyric + propionic acids

Butyric acid – H_2O (revised)
Butyric acid – propionic acid – H_2O (revised)
Calcium butanoate – H_2O (revised)
Potassium butanoate – H_2O (revised)

NH_3 + K_2CO_3 + MDEA and related systems

NH_3 – K_2CO_3 – H_2O (revised)
NH_3 – K_2CO_3 – $(NH_4)_2CO_3$ – H_2O (revised)
MDEA – K_2CO_3 – H_2O
MDEA – NH_3 – K_2CO_3 – H_2O
MDEA – CO_2 – K_2CO_3 – H_2O
MDEA – K_2CO_3 – CO_2 – NH_3 – H_2O
MDEA – NH_3 – H_2O
MDEA – CO_2 – NH_3 – H_2O
MDEA – NH_4HCO_3 – H_2O
MDEA – NH_3 – NH_4HCO_3 – H_2O

Piperazine + CO_2 +H_2S +H_2O + MDEA

Piperazine – H_2O
Piperazine – CO_2 – H_2O
Piperazine – MDEA – H_2O
Piperazine – CO_2 – MDEA – H_2O
Piperazine – H_2S – H_2O
Piperazine – H_2S – MDEA – H_2O

Revision of properties of selenium species: Se^0 and SeO_4^{2-}

Se – NaCl – H_2O

Crystalline calcium silicates moved from CRMSE databank to GEMSE

Afwillite, $Ca_3Si_2O_4(OH)_6$
Foshagite, $Ca_4Si_3O_9(OH)_2.0.5H_2O$
Gyrolite, $Ca_2Si_3O_7(OH)_2.1.5H_2O$
Hatrurite, Ca_3SiO_5

Hillebrandite, $Ca_2SiO_3(OH)_2.0.17H_2O$
Okenite, $CaSi_2O_4(OH)_2.H_2O$
Rankinite, $Ca_3Si_2O_7$
Tobermorite11A, $Ca_5Si_6H_{11}O_{22.5}$
Tobermorite14A, $Ca_5Si_6H_{21}O_{27.5}$
Tobermorite9A, $Ca_5Si_6H_6O_{20}$
Xonotlite, $Ca_6Si_6O_{17}(OH)_2$
Clinochrysotile, $Mg_3Si_2O_5(OH)_4$

Cobalt chemistry: $CoSO_4$ $(NH_4)_2SO_4$, $Ni_{0.78}Co_{0.22}(NH_4)_2(SO_4)_2$, Co-$NH_3$ complexes

$(NH_4)_2SO_4$ – $CoSO_4$ – H_2O
$CoSO_4(NH_4)_2SO_4$ – H_2O
$NiSO_4(NH_4)_2SO_4$ – $CoSO_4(NH_4)_2SO_4$ – H_2O
System where $Ni_{0.78}Co_{0.22}(SO_4)_2(NH_4)_2 \cdot 6H_2O$ precipitates

$MnSO_4$ + $(NH_4)_2SO_4$ + H_2O

$MnSO_4$ – $(NH_4)_2SO_4$ – H_2O

Nd citrate entropy and Cp: correction

Al phosphates

$AlPO_4$ – H_3PO_4 – H_2O
Al_2O_3 – P_2O_5 – H_2O

NH_4 phosphates

$NH_4H_2HPO_4$ – NH_3 – H_3PO_4 – H_2O
$(NH_4)_2HPO_4$ – NH_3 – H_3PO_4 – H_2O
$(NH_4)_2HPO_4 \cdot 2H_2O$– NH_3 – H_3PO_4 – H_2O
$(NH_4)_3PO_4 \cdot 3H_2O$– NH_3 – H_3PO_4 – H_2O

Mn phosphates

MnO – P_2O_5 – H_2O
$Mn_3(PO_4)_2$ – H_3PO_4 – H_2O

Fe phosphates

$FePO_4$ – H_2O
$FePO_4$ – H_3PO_4 – H_2O

Zn phosphates

$Zn_3(PO_4)_2$ – H_3PO_4 – H2O

Na_2HPO_4 + $NaNO_3$ + H_2O

Na_2HPO_4 – $NaNO_3$ – H_2O

H_3BO_3 + sulfates (Na, K, Li, Mg, Ca)

H_3BO_3 – Na_2SO_4 – H_2O
H_3BO_3 – K_2SO_4 – H_2O
H_3BO_3 – Li_2SO_4 – H_2O
H_3BO_3 – $MgSO_4$ – H_2O
H_3BO_3 – $CaSO_4$ – H_2O
HBO_2 (aq, vap) removed – only HBO_2(s) remains

Rare earth element hydroxycarbonates, carbonates and REE fluorocarbonates

$YOHCO_3 – (CO_2) – H_2O$
$LaOHCO_3 – (CO_2) – H_2O$
$CeOHCO_3 – (CO_2) – H_2O$
$PrOHCO_3 – (CO_2) – H_2O$
$NdOHCO_3 – (CO_2) – H_2O$
$SmOHCO_3 – (CO_2) – H_2O$
$EuOHCO_3 – (CO_2) – H_2O$
$GdOHCO_3 – (CO_2) – H_2O$
$TbOHCO_3 – (CO_2) – H_2O$
$DyOHCO_3 – (CO_2) – H_2O$
$HoOHCO_3 – (CO_2) – H_2O$
$ErOHCO_3 – (CO_2) – H_2O$
$TmOHCO_3 – (CO_2) – H_2O$
$YbOHCO_3 – (CO_2) – H_2O$
$LuOHCO_3 – (CO_2) – H_2O$

$Y_2(CO_3)_3 – H_2O$
$La_2(CO_3)_3 – H_2O$
$Ce_2(CO_3)_3 – H_2O$
$Pr_2(CO_3)_3 – H_2O$
$Nd_2(CO_3)_3 – H_2O$
$Sm_2(CO_3)_3 – H_2O$
$Eu_2(CO_3)_3 – H_2O$
$Gd_2(CO_3)_3 – H_2O$
$Tb_2(CO_3)_3 – H_2O$
$Dy_2(CO_3)_3 – H_2O$
$Ho_2(CO_3)_3 – H_2O$
$Er_2(CO_3)_3 – H_2O$
$Tm_2(CO_3)_3 – H_2O$
$Yb_2(CO_3)_3 – H_2O$
$Lu_2(CO_3)_3 – H_2O$

$YFCO_3 – H_2O$
$LaFCO_3 – H_2O$
$CeFCO_3 – H_2O$
$PrFCO_3 – H_2O$
$NdFCO_3 – H_2O$
$SmFCO_3 – H_2O$
$EuFCO_3 – H_2O$
$GdFCO_3 – H_2O$
$TbFCO_3 – H_2O$
$DyFCO_3 – H_2O$
$HoFCO_3 – H_2O$
$ErFCO_3 – H_2O$
$TmFCO_3 – H_2O$
$YbFCO_3 – H_2O$
$LuFCO_3 – H_2O$

Rare earth element oxyfluorides and oxychlorides

$YOCl – H_2O$
$LaOCl – H_2O$
$CeOCl – H_2O$
$PrOCl – H_2O$
$NdOCl – H_2O$

SmOCl – H_2O
EuOCl – H_2O
GdOCl – H_2O
TbOCl – H_2O
DyOCl – H_2O
HoOCl – H_2O
ErOCl – H_2O
TmOCl – H_2O
YbOCl – H_2O
LuOCl – H_2O
YOF – H_2O
LaOF – H_2O
CeOF – H_2O
PrOF – H_2O
NdOF – H_2O
SmOF – H_2O
EuOF – H_2O
GdOF – H_2O
TbOF – H_2O
DyOF – H_2O
HoOF – H_2O
ErOF – H_2O
TmOF – H_2O
YbOF – H_2O
LuOF – H_2O

Crystalline rare earth hydroxides moved from MSEPUB to GEMSE and CRMSE

$Y(OH)_3cr$
$La(OH)_3cr$
$Ce(OH)_3cr$
$Pr(OH)_3cr$
$Nd(OH)_3cr$
$Sm(OH)_3cr$
$Eu(OH)_3cr$
$Gd(OH)_3cr$
$Tb(OH)_3cr$
$Dy(OH)_3cr$
$Ho(OH)_3cr$
$Er(OH)_3cr$
$Tm(OH)_3cr$
$Yb(OH)_3cr$
$Lu(OH)_3cr$

Lithium chemistry (Li + Na + K + Cl + SO_4 + H_2O) (revision)

Na_2SO_4 – Li_2SO_4 – H_2O
NaCl – LiCl – H_2O
Li_2SO_4 – Na_2SO_4 – K_2SO_4 – H_2O
$LiNO_3$ – KNO_3 – H_2O
Li_2SO_4 – K_2SO_4 – H_2O
LiCl – KCl – H_2O
Li_2SO_4 – H_2O density
Li_2SO_4 – LiCl – H_2O
Li_2SO_4 – K_2SO_4 – H_2O
Li_2SO_4 – $MgSO_4$ – H_2O
Li_2SO_4 (LiCl) – $CaSO_4$($CaCl_2$) – H_2O

Li_2SO_4 – $MnSO_4$ – H_2O
Li_2SO_4 – $CoSO_4$ – H_2O
Li_2SO_4 – $(NH_4)_2SO_4$ – H_2O
Li_2SO_4 – $NiSO_4$ – H_2O

Co hydrolyzed species – conventional and non-conventional species

$Co(OH)_2$ – H_2O
$Co(OH)_2$ – NaOH(KOH) – H_2O
$Co(OH)_2$ – HCl – H_2O

EuO + H_2O

EuO – NaOH – H_2O

$LiBF_4$ + organic carbonates

$LiBF_4$ – Dimethyl carbonate (Lithium tetrafluoroborate hemidimethyl carbonate, Lithium tetrafluoroborate dimethyl carbonate)

Co and Ni solvent extraction chemistry

CYANEX272 – H_2O
CYANEX301 – H_2O
DEHPA – H_2O
PC88A – H_2O
VERSATIC10 – H_2O
Co and Ni extraction using CYANEX272 extractant and isooctane as solvent
Co and Ni extraction using CYANEX272 extractant and high boiling kerosene (KEROSENE) as solvent
Co and Ni extraction using CYANEX272 extractant and low boiling kerosene (KEROSENUN) as solvent in the presence of Tributyl phosphate (TRIBUTPHOS)
Co and Ni extraction using CYANEX272 extractant and Toluene as solvent
Co extraction using CYANEX272 extractant and n-Heptane as solvent
Co extraction using PC88A extractant and n-Heptane as solvent
Co and Ni extraction using D2EHPA extractant and low boiling kerosene (KEROSENUN) as solvent in the presence of Tributyl phosphate (TRIBUTPHOS)
Li and Co extraction using D2EHPA extractant and high boiling kerosene (KEROSENE) as solvent
Li, Co, and Ni extraction using PC88A extractant and high boiling kerosene (KEROSENE) as solvent
Li, Co, and Ni extraction using PC88A extractant and low boiling kerosene (KEROSENUN) as solvent
Li, Co, and Ni extraction using PC88A extractant and low boiling kerosene (KEROSENUN) as solvent in the presence of Tributyl phosphate (TRIBUTPHOS)

$MnCO_3$ and $Mn(ClO_4)_2$ systems

$MnCO_3$ – NaCl – $NaClO_4$ – Na_2CO_3 – H_2O
$MnCO_3$ – NaCl – $NaClO_4$ – HCl – H_2O

$MgCl_2$ – adding anhydrous species

$MgCl_2$ – H_2O

KOH revision + related systems

KOH – H_2O (revised)
KOH – Ag_2O – H_2O (tested)
KOH – $Be(OH)_2$ / BeO – H_2O (tested)
KOH – CH_4 – H_2O (tested)
KOH – GaOOH – H_2O including potassium gallate (tested)
KOH – H_3BO_3 – H_2O including potassium borates (tested)
KOH – Np(IV) – K_2CO_3 ($KHCO_3$) – H_2O (tested)
KOH – $PbCO_3$ – CO_2 ($KHCO_3$) – H_2O (tested)

KOH – Pu(IV) – K_2CO_3 ($KHCO_3$) – H_2O (tested)
KOH – tannic acid – H_2O (tested)
KOH – U(IV) –K_2CO_3($KHCO_3$) – H_2O (tested)
KOH – ZnO – H_2O (tested)
KOH (K_2O) – B_2O_3 – H_2O (revised)
KOH – $Zn(OH)_2$ / ZnO – H_2O (revised)

Density of $NaHCO_3$ + H_2O and $NaHCO_3$ + Na_2CO_3 + H_2O

$NaHCO_3$ – H_2O
$NaHCO_3$ – Na_2CO_3 – H_2O

KBr + H_2O

KBr – H_2O

$Ca(OH)_2$ + NaOH and LiOH + H_2O

$Ca(OH)_2$ – NaOH – H_2O
$Ca(OH)_2$ – LiOH – H_2O

Cl_2 – HCl – chloride salts

Cl_2 – HCl – H_2O
Cl_2 – NaCl – H_2O
Cl_2 – KCl – H_2O
Cl_2 – $MgCl_2$ – H_2O
Cl_2 – $CaCl_2$ – H_2O
Cl_2 – $SrCl_2$ – H_2O
Cl_2 – $BaCl_2$ – H_2O
Cl_2 – $NiCl_2$ – H_2O
Cl_2 – H_2SO_4 – H_2O

Transport properties

Cl_2 (HClO) – H_2O	(revised, electrical conductivity)
LiCl – H_2O	(revised, electrical conductivity)
LiCl – H_2O	(thermal conductivity)
LiCl – H_2O	(revised, viscosity)
LiCl – methanol – H_2O	(revised, electrical conductivity)
KOH – H_2O	(revised, electrical conductivity)
KOH – H_2O	(thermal conductivity)
KOH – H_2O	(revised, viscosity)
KOH – ZnO – H_2O	(electrical conductivity)

Scaling inhibition kinetics

$SrSO_4$	(revised)
$BaSO_4$	(revised)
$CaSO_4 \cdot 2H_2O$	(revised)
$CaCO_3$ (Calcite)	(revised)
SrSO4-HEDP	(revised)
SrSO4-DTPMP	(revised)

BaSO4-HEDP (revised)
BaSO4-NTMP (revised)
BaSO4-DTPMP (revised)

$CaSO_4{\cdot}2H_2O$-HEDP (revised)
$CaSO_4{\cdot}2H_2O$-NTMP (revised)
$CaSO_4{\cdot}2H_2O$-DTPMP (revised)
$CaSO_4{\cdot}2H_2O$-EDTMP
$CaSO_4{\cdot}2H_2O$-PBTC (revised)

$CaCO_3$(Calcite)-HEDP (revised)
$CaCO_3$(Calcite)-NTMP (revised)
$CaCO_3$(Calcite)-DTPMP (revised)
$CaCO_3$(Calcite)-PMLA (revised)

HEDP: 1-hydroxyethane 1,1-diphosphonic acid
NTMP: Nitrilotris(methylenephosphoric acid)
DTPMP: Diethylenetriamine penta(methylene phosphonic acid)
EDTMP: Ethylenediamine tetra(methylene phosphonic acid)
PBTC: 2-phosphono-butane-1,2,4-tricarboxylic acid
PMLA: Poly maleic acid

MSE Corrosion: Electrochemical kinetics databank

MSE Alloy 2507

Corrosive environments:

- NaCl
- Seawater – O_2
- $MgCl_2$ – NaCl
- NaCl – O_2
- H_2S – NaCl
- CO_2 – NaCl
- CO_2 – H_2S – NaCl
- NaCl – acetic acid – H_2S – CO_2
- NaOH
- *NaOH – NaCl*
- Formic acid
- Acetic acid
- Formic acid - acetic acid
- H_2SO_4
- HCl
- HNO_3
- H_3PO_4
- HCl – H_2SO_4
- HCl – HNO_3
- HF
- H_2SO_4 – HNO_3
- *HCl – H_3PO_4*
- *HNO_3 – H_3PO_4*
- *H_2SO_4 – HF*
- HF – HNO_3
- HF – H_3PO_4
- *HCl – HF*

$HBr – H_3PO_4$
H_2SO_4 – acetic acid
H_2SO_4 –formic acid
NaCl – acetic acid
NaCl –formic acid
$CuCl_2$
$FeCl_3$
$FeCl_3 – FeCl_2 – NaCl – HCl$
$CuCl_2 – CuCl – NaCl – HCl$
$H_2SO_4 – Fe_2(SO_4)_3$
$H_2SO_4 – Fe_2(SO_4)_3 – NaCl$

Repassivation potential parameters:

Cl^-
H_2S
SO_4^{2-}
NO_3^-
OH^-
VO_4^{3-}
MoO_4^{2-}
NO_2^-

MSE Alloy 2205

Corrosive environments:

NaCl
Seawater – O_2
$MgCl_2 – NaCl$
$NaCl – O_2$
$H_2S – NaCl$
$CO_2 – NaCl$
$CO_2 – H_2S – NaCl$
$NaCl$ – acetic acid – $H_2S – CO_2$
NaOH
NaOH – NaCl
Formic acid
Acetic acid
Formic acid - acetic acid
H_2SO_4
HCl
HNO_3
H_3PO_4
$HCl – H_2SO_4$
$HCl – HNO_3$
HF
$H_2SO_4 – HNO_3$
$HCl – H_3PO_4$
$HNO_3 – H_3PO_4$
$H_2SO_4 – HF$
$HF – HNO_3$
$HF – H_3PO_4$
HCl – HF
$HBr – H_3PO_4$
H_2SO_4 – acetic acid

H_2SO_4 –formic acid
NaCl – acetic acid
NaCl –formic acid
$CuCl_2$
$FeCl_3$
$FeCl_3$ – $FeCl_2$ – NaCl – HCl
$CuCl_2$ – CuCl – NaCl – HCl
H_2SO_4 – $Fe_2(SO_4)_3$
H_2SO_4 – $Fe_2(SO_4)_3$ – NaCl

Repassivation potential parameters:

Cl^-
H_2S
SO_4^{2-}
NO_3^-
OH^-
VO_4^{3-}
MoO_4^{2-}
NO_2^-

Aqueous (AQ) thermophysical property databank

Crystalline calcium silicates moved from the CORROSION databank to GEOCHEM:

Afwillite, $Ca_3Si_2O_4(OH)_6$
Foshagite, $Ca_4Si_3O_9(OH)_2.0.5H_2O$
Gyrolite, $Ca_2Si_3O_7(OH)_2.1.5H_2O$
Hatrurite, Ca_3SiO_5
Hillebrandite, $Ca_2SiO_3(OH)_2.0.17H_2O$
Okenite, $CaSi_2O_4(OH)_2.H_2O$
Rankinite, $Ca_3Si_2O_7$
Tobermorite11A, $Ca_5Si_6H_{11}O_{22.5}$
Tobermorite14A, $Ca_5Si_6H_{21}O_{27.5}$
Tobermorite9A, $Ca_5Si_6H_6O_{20}$
Xonotlite, $Ca_6Si_6O_{17}(OH)_2$
Clinochrysotile, $Mg_3Si_2O_5(OH)_4$

AQ Corrosion: Electrochemical kinetics databank

AQ Alloy 304 – revision

Corrosive environments:

O_2
NaCl – O_2
Seawater – O_2
$MgCl_2$ – O_2
Na_2SO_4 – O_2
NaCl – HF – O_2
HF– O_2
H_2O_2 – H_2 – O_2
H_2O_2 – H_2 – O_2 – NaCl – $FeCl_3$
Cl_2 – O_2

$NaOH - O_2$
$LiOH - O_2$
$B(OH)_3 - O_2$

AQ Alloy 316 – revision

Corrosive environments:

$NaCl$
HCl
$HCl - HNO_3$
$HCl - H_3PO_4$
$HCl - H_2SO_4$
$FeCl_3$
$FeCl_2$
$CuCl_2$
$CuCl$

AQ Alloy 2205 – revision

Corrosive environments:

O_2
HF
$Seawater - O_2$
$NaCl - O_2$
$NaOH - O_2$

AQ Alloy 2507 – revision

Corrosive environments:

O_2
HF
$NaCl\text{-}NaF\text{-}O_2$
$Seawater - O_2$
$NaCl - O_2$
$NaOH - O_2$
H_3PO_4 - HF