

# OLI Software 9.5.3

## What is new?

March 6, 2017

### Mixed-solvent electrolyte databanks:

#### MSEPUB

##### *New systems:*

##### Lead chemistry

PbMoO<sub>4</sub> (wulfenite) – HClO<sub>4</sub>, HNO<sub>3</sub>  
Pb acetate – acetic acid  
Pb formate  
Pb(NO<sub>3</sub>)<sub>2</sub> – HNO<sub>3</sub>

##### Rare-earth metal chemistry

Nd<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub>, NdHCO<sub>3</sub> – CO<sub>2</sub>  
YCl<sub>3</sub> - HCl

##### Iron chemistry

FeCl<sub>3</sub> - NaCl

##### NO<sub>x</sub> chemistry

NO<sub>2</sub> – H<sub>2</sub>O – HNO<sub>3</sub>  
NO<sub>2</sub> – CO<sub>2</sub>  
N<sub>2</sub>O<sub>3</sub> – H<sub>2</sub>O  
N<sub>2</sub>O<sub>3</sub> – CO<sub>2</sub>  
NO – H<sub>2</sub>O  
NO – CO<sub>2</sub>  
N<sub>2</sub>O – H<sub>2</sub>O  
N<sub>2</sub>O – CO<sub>2</sub>

##### SO<sub>2</sub> chemistry

SO<sub>2</sub> – CO<sub>2</sub>

##### Silver chemistry

AgNO<sub>3</sub> – HNO<sub>3</sub> – H<sub>2</sub>O  
Ag<sub>2</sub>SO<sub>4</sub> – H<sub>2</sub>SO<sub>4</sub> – H<sub>2</sub>O

##### C-H-N chemistry

Melamine  
Melam  
Ammeline  
Ammelide  
Cyanuric acid

##### Ammonia properties

Viscosity, thermal conductivity

Bromide chemistry

NaBr

Lithium chemistry

Li<sub>2</sub>SO<sub>4</sub>

LiAl(SiO<sub>3</sub>)<sub>2</sub> (spodumene)

Zinc chemistry

ZnCl<sub>2</sub> - NaCl

Silicate chemistry

Ca silicates

Ca<sub>5</sub>Si<sub>6</sub>O<sub>17</sub>·5.5H<sub>2</sub>O (amorphous tobermorite)

Ca<sub>3</sub>Si<sub>2</sub>O<sub>7</sub>·3H<sub>2</sub>O (amorphous afwillite)

Mg silicates

Mg<sub>4</sub>[Si<sub>6</sub>O<sub>15</sub>(OH)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]·4H<sub>2</sub>O (amorphous sepiolite)

Mg<sub>3</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub> (amorphous antigorite)

Mg<sub>3</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub> (poorly-crystalline antigorite)

Ca – Na silicates

NaCa<sub>2</sub>Si<sub>3</sub>O<sub>8</sub>(OH) (pectolite)

Ca(HCO<sub>3</sub>)<sub>2</sub> (general information only)

**Revised systems:**

FeCO<sub>3</sub> chemistry

FeCO<sub>3</sub> – CO<sub>2</sub> – H<sub>2</sub>O

FeCO<sub>3</sub> – NaCl – H<sub>2</sub>O

FeCO<sub>3</sub> – NaClO<sub>4</sub> – H<sub>2</sub>O

FeS (troilite, mackinawite) chemistry

FeS – H<sub>2</sub>S – H<sub>2</sub>O

FeS – NaHS – H<sub>2</sub>O

FeS – NaCl – H<sub>2</sub>O

Iron chloride chemistry

FeCl<sub>2</sub> – HCl

FeCl<sub>3</sub> – HCl

Pu(V) chemistry

Pu(V) – NaOH

PuO<sub>2</sub>OH, Na<sub>2</sub>PuO<sub>2</sub>(OH)<sub>3</sub>·2H<sub>2</sub>O, NaPuO<sub>2</sub>(OH)<sub>2</sub>

Pu(VI) chemistry

Pu(VI) – NaClO<sub>4</sub>, HClO<sub>4</sub>, NaOH

PuO<sub>2</sub>(OH)<sub>2</sub>·H<sub>2</sub>O

Pu(VI) – CO<sub>2</sub>, LiHCO<sub>3</sub>, NaClO<sub>4</sub>, NaCl, (NH<sub>4</sub>)<sub>4</sub>CO<sub>3</sub>

PuO<sub>2</sub>CO<sub>3</sub>

Np(V) chemistry

Np(V) – HCl, NaOH, NaClO<sub>4</sub>, NaNO<sub>2</sub>, NaNO<sub>3</sub>  
NpO<sub>2</sub>OH  
Np(V) - CO<sub>2</sub>, NaClO<sub>4</sub>, NaCl, Na<sub>2</sub>CO<sub>3</sub>, NaNO<sub>3</sub>, KCl  
NaNpO<sub>2</sub>CO<sub>3</sub>·3.5H<sub>2</sub>O, Na<sub>3</sub>NpO<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>

#### Np(VI) chemistry

Np(VI) – NaCl, NaOH  
NpO<sub>2</sub>(OH)<sub>2</sub>·H<sub>2</sub>O, Na<sub>2</sub>Np<sub>2</sub>O<sub>7</sub>  
Np(VI) – CO<sub>2</sub>, NaClO<sub>4</sub>, NaCl  
NpO<sub>2</sub>CO<sub>3</sub>

#### Sr chemistry

SrSO<sub>4</sub> – H<sub>2</sub>O  
SrSO<sub>4</sub> – NaCl  
SrSO<sub>4</sub> – Na<sub>2</sub>SO<sub>4</sub>  
SrSO<sub>4</sub> – KCl  
SrSO<sub>4</sub> – MgCl<sub>2</sub>  
SrSO<sub>4</sub> – CaCl<sub>2</sub>  
SrCO<sub>3</sub> – H<sub>2</sub>O – CO<sub>2</sub>  
SrCO<sub>3</sub> – NaCl  
SrCO<sub>3</sub> – KCl

#### Lithium chemistry

Li<sub>2</sub>CO<sub>3</sub>

#### Calcium chemistry

Ca(OH)<sub>2</sub>

#### Hydrocarbon chemistry

CH<sub>4</sub> – CO<sub>2</sub> – H<sub>2</sub>O  
H<sub>2</sub>S – hydrocarbon mixtures  
CH<sub>4</sub> – hydrocarbon mixtures  
Ethane  
Propane  
Butane  
Pentane  
Hexane  
Heptane  
Octane  
Nonane  
Decane  
Undecane  
Dodecane  
Tridecane  
Tetradecane  
Pentadecane  
Hexadecane  
Heptadecane  
Octadecane  
Eicosane  
Docosane  
Tetracosane  
Octacosane  
Triacontane

Dotriacontane  
Hexatriacontane  
Isobutane  
Isopentane  
Neopentane  
Isooctane  
Ethylene  
Propylene  
Cyclohexane  
Benzene  
Toluene  
Meta-xylene  
Naphthalene  
Phenanthrene

Correlations for pseudocomponents with H<sub>2</sub>S and CH<sub>4</sub>

Viscosity

C<sub>40</sub>H<sub>82</sub>

Volume of solids

KMgCl<sub>3</sub>·6H<sub>2</sub>O

## **GEMSE**

Ca<sub>5</sub>Si<sub>6</sub>O<sub>17</sub>·5.5H<sub>2</sub>O (tobermorite-like CSH)

Eliminated Zn(OH)<sub>2</sub> and CuO

## **CRMSE**

Eliminated CuO

## **XSCDLM (surface complexation):**

**Surface complexation on FeOOH:**

SeO<sub>4</sub>

Pb

Cd

Zn

Cu

Ag

Co

Cr

Cr

AsO<sub>4</sub>

Hg

CrO<sub>4</sub>

Ni

Sr

Ba

Ca

VO<sub>4</sub>

H<sub>3</sub>AsO<sub>3</sub>

H<sub>3</sub>BO<sub>3</sub>

## **Aqueous databanks:**

### **PUBLIC:**

#### *New systems:*

Ca(HCO<sub>3</sub>)<sub>2</sub> (general information only)

#### *Revised:*

CaCO<sub>3</sub> – CaCl<sub>2</sub>

### **SCDLM (surface complexation):**

#### **Surface complexation on FeOOH:**

SeO<sub>4</sub>

Pb

Cd

Zn

Cu

Ag

Co

Cr

Cr

AsO<sub>4</sub>

Hg

CrO<sub>4</sub>

Ni

Sr

Ba

Ca

VO<sub>4</sub>

H<sub>3</sub>AsO<sub>3</sub>

H<sub>3</sub>BO<sub>3</sub>