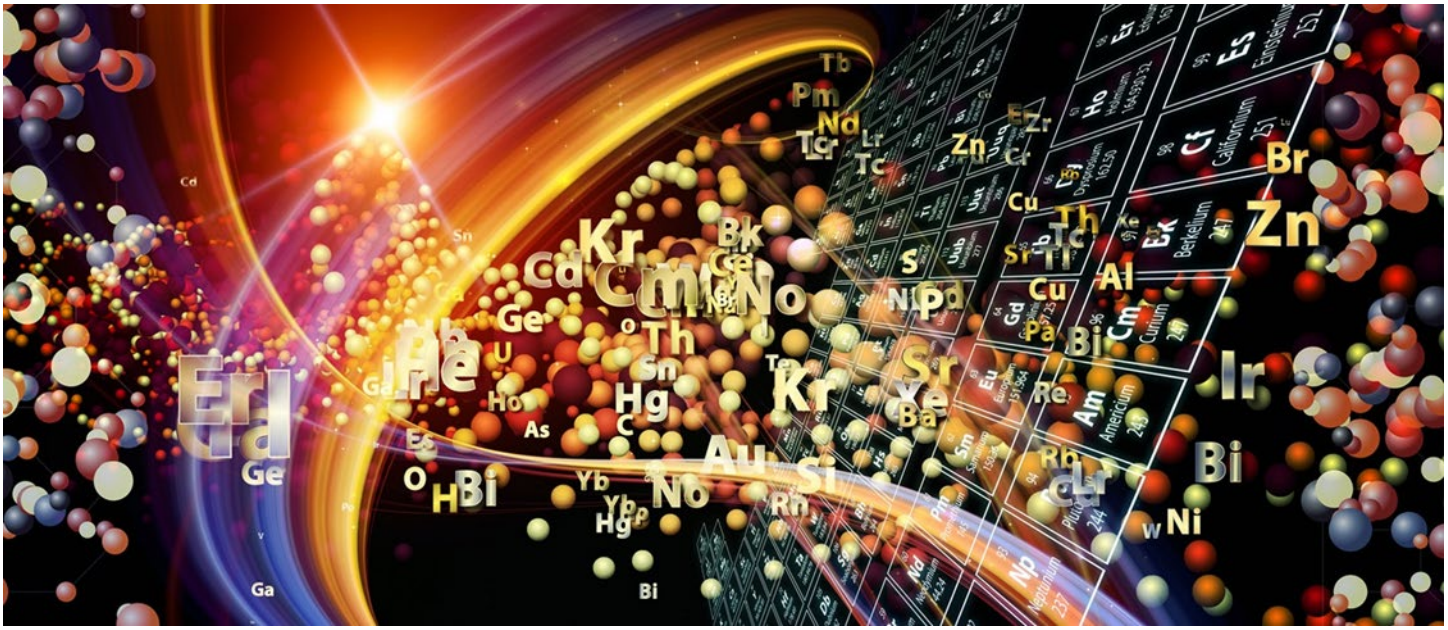

OLI Software Release Notes V10

Jim Berthold

6/8/20

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Introduction

For many years, the OLI software release notes were maintained on several different web pages. While this was suitable at the time it has become far too cumbersome to maintain.

With the release of OLI Software V9.6 the release notes have been combined into a single document.

Each version will be listed in reverse chronological order. Within each version update to the products will be listed in this order:

- Databank updates
- Databank fixes
- Engine/solver
- OLI Studio/Analyzer
- OLI Flowsheet: ESP
- OLI Chemistry Wizard
- OLI Developer Edition
- OLI Alliance products
    - Aspen Hysys
    - Aspen Plus
    - gProms
    - IDEAS
    - Petro-Sim
    - ProII
    - Unisim Design
- OLI Security/License Manager

Version 10.0.2

General Information

The databanks were released on the same date as the first product. All engine/solver updates were included on the same date as the first release.

Product	Release Date
OLI Studio/Analyzer	June 8, 2020
OLI Flowsheet: ESP / ESP FS[1]	June 8, 2020
Chemistry Wizard	June 8, 2020
OLI Developer Edition	June 8, 2020
OLI Engine 10.x for Aspen Hysys	June 8, 2020
OLI Engine 10.x for Aspen Plus	June 8, 2020
OLI Engine 10.x for Petro-Sim	June 8, 2020
OLI Engine 10.x for ProII	June 8, 2020
OLI Engine 10.x for Unisim Design	June 8, 2020
OLI License Manager[2]	June 8, 2020

OLI Engine 10.x for gProms was not updated for this release

OLI Engine 10.x for IDEAS was not updated for this release

[1] The product ESP FS is for Asia releases. It is functionally identical to OLI Flowsheet: ESP.

[2] This product does not follow the same versioning scheme as the other products. The current version is 4.0.1.18

Databank Updates

Mixed-solvent electrolyte (MSE) databank

MSEPUB

Sr chemistry - revision

$SrSO_4$ – NaCl

$SrSO_4$ – Na_2SO_4

$SrSO_4$ – KCl

$SrSO_4$ – $MgCl_2$

$SrSO_4$ – $MgCl_2$ - NaCl

$SrSO_4$ – $CaCl_2$

$SrSO_4$ – $CaCl_2$ – NaCl

$SrSO_4$ – $CaCl_2$ – $MgCl_2$ – NaCl

Glycol chemistry - revision

Monoethylene glycol – N_2

Monoethylene glycol – O_2

Hg chemistry

Hg – N_2

Fe chemistry - revision

$FeSO_4$

Potash chemistry – revision of diffusion coefficients only

NaCl

KCl

$MgCl_2$

Na_2SO_4

NaCl – HCl

NaCl – KCl

$NaCl – MgCl_2$

$NaCl – MgCl_2 – CaCl_2$

NaCl - MeOH

$Na – K – Mg – Ca – Cl – SO_4$

OLI Databook – Bugs

Bug ID	Problem	Resolution
2964	OLI Databook prompts for password when there is none	If no password is used, none are prompted
2998	When opening a databank, the corresponding public databank is not opened	Databank properly opened

Engine/Solver - Features

Bug ID	AREA	Problem	Resolution
3569	Solver	Change default ppt calculation value to 1.e-12	Some mineral systems have solids with very small solubilities. Less than the default 1E-08 mol/Kg. The regression of the data allowed for these small solubilities, but the solver did not. This new parameter accounts for these small soluble solids.

Engine/Solver - Bugs

Bug ID	AREA	Problem	Resolution
2737	Solver	HF Alkylation convergence issue	Stiff numerical system.
2753	Solver	Incorrect phase prediction - wrong label	Engine updated to use smarter logic to report a phase.

OLI Studio/Analyzer - Features

Bug ID	AREA	Problem	Resolution
		No Features added for this build	

OLI Studio/Analyzer - Bugs

Bug ID	AREA	Problem	Resolution
2878	ALL	4K screen causes a shrinkage on OLI Studio Resolution	Install manifest now ignores 4K resolution.

OLI Flowsheet: ESP / ESP-FS - Features

Bug ID	AREA	Problem	Resolution
		No Features added for this build	

OLI Flowsheet: ESP / ESP-FS - Bug

Bug ID	AREA	Problem	Resolution
2279	Engine	Heat Exchanger- Vapor Fraction calculation type not working	This calculation is now supported
2491	Engine	Invalid block order when using a Virtual Stream	Block order calculation logic improved.
2594	Engine	CRASH: Error message, the solver exited in an unexpected manner. Need better resolution	Logic and text were updated to provide better meaning.
2579	Engine	Volumetric stream converged with unreasonable aqueous phase using HF private databank in Flowsheet	The data was incorrect, but it could have been checked prior to execution.
2794	Engine	Block order failure with duplicate names	It is possible to enter blocks with the same name. This confuses the block order calculation. The engine checks for duplicate names and sends a warning to the interface.
2906	Engine	Non-converged HX block. No real warnings (possible failure in approach temperature)	The block truly did not converge but the warnings were misleading. The text and logic were improved

Alliance Products - Features

Bug ID	Program	Problem	Resolution
		No Features added for this build	

Alliance Products - Bugs

Bug ID	Program	Problem	Resolution
2741	Petro-Sim	KBC column converge with 0 outflow	Output arrays not properly aligned
2853	Petro-Sim		
2887	Petro-Sim	HYPFRC is not honoring resfil parameter for restart KBC PetroSim	File names updated to account for unit operation name

OLI Chemistry Wizard (all products)

Bug ID	Program	Problem	Resolution
2995	All	4K Screen causes OLI Chemistry Wizard display issues	Install manifest now ignores 4K resolution.

OLI Developer Edition - General

Bug ID	Program	Problem	Resolution
2991	API	Add Custom calculation support to OLI EngineAPI	Custom calculation support added

OLI Framework - General

Bug ID	Program	Problem	Resolution
		No Features added for this build	

Version 10.0.1

General Information

The databanks were released on the same date as the first product. All engine/solver updates were included on the same date as the first release.

Product	Release Date
OLI Studio/Analyzer	November 1, 2019
OLI Flowsheet: ESP / ESP FS[3]	November 1, 2019
Chemistry Wizard	November 1, 2019
OLI Developer Edition	November 1, 2019
OLI Engine 10.x for Aspen Hysys	November 1, 2019
OLI Engine 10.x for Aspen Plus	November 1, 2019
OLI Engine 10.x for ProII	November 1, 2019
OLI Engine 10.x for Unisim Design	November 1, 2019
OLI License Manager[4]	November 1, 2019

OLI Engine 10.x for gProms was not updated for this release

OLI Engine 10.x for IDEAS was not updated for this release

[3] The product ESP FS is for Asia releases. It is functionally identical to OLI Flowsheet: ESP.

[4] This product does not follow the same versioning scheme as the other products. The current version is 4.0.1.17

Databank Updates

MSE model

Se(VI) chemistry

- Selenic acid chemistry
  - H_2SeO_4 – SeO_3 - H_2O including
  - $H_2SeO_4 \cdot SeO_3$
  - $2H_2SeO_4 \cdot SeO_3$
- Sodium selenate/biselenate chemistry
  - Na_2SeO_4 – SeO_3 - H_2O including
  - $NaHSeO_4$
  - Na_2SeO_4
  - $Na_2SeO_4 \cdot 2H_2SeO_4$
  - $2Na_2SeO_4 \cdot 3H_2SeO_4$
- Magnesium selenate chemistry
  - $MgSO_4$ – SeO_3 – H_2O including
  - $MgSeO_4$
  - $MgSeO_4 \cdot H_2SeO_4$
- $ZnSeO_4$ – H_2O
- $MnSeO_4$ – H_2O
- $PbSeO_4$ – H_2O
- $Fe_2(SeO_4)_3$ – H_2O
- $FeSeO_4$ – H_2O

Se(IV) chemistry

- SeO_2 - H_2SeO_2 – H_2O
- Sodium selenite/biselenite chemistry including
  - Na_2SeO_3 – H_2O
  - Na_2SeO_3 – Na_2CO_3 - H_2O
  - $Na_2Se_2O_5$
  - $NaHSeO_3$ – H_2O
  - $NaH_3(SeO_3)_2$ – H_2O
  - $MgSeO_3$ – H_2O
  - $MnSeCO_3$ – H_2O
  - $ZnSeO_3$ – H_2O
  - $Fe_2(SeO_3)_3$ – H_2O
  - $Fe_2(SeO_3)_3$ – Na_2CO_3 - H_2O

Se(II) chemistry

- H_2Se – H_2O
- Na_2Se – $NaOH$ – H_2O
- As_2Se_3
- Sb_2Se_3
- $ZnSe$
- $PbSe$
- Cu_2Se
- $CuSe$
- $FeSe$
- $MnSe$

$MnSe_2$
$MoSe_2$
NiSe
SnSe
$SnSe_2$

Se(0)

Sulfur dioxide chemistry

$SO_2 – NH_3 – H_2O$ including
$(NH_4)_2SO_3$, NH_4HSO_3, $(NH_4)_2S_2O_5$

Gallic acid chemistry

Gallic acid – H_2O
Gallic acid – NaCl – H_2O
Gallic acid – KCl – H_2O
Gallic acid – LiCl – H_2O

Tannic acid chemistry

Tannic acid – H_2O
Tannic acid – KOH – H_2O

Fulvic acid chemistry

Fulvic acid – H_2O
Fulvic acid as a function of pH (titrated with NaOH) with KNO_3, $NaClO_4$, KCl
Fulvic acid complexation with
- As(V)
- As(III)
- Ca
- Co
- Cu
- Fe(II)
- Mg
- Mn
- Ni
- Pb
- Zn

Humic acid chemistry

Humic acid – H_2O
Humic acid as a function of pH (titrated with NaOH, KOH) with NaCl, KNO_3, HCOOH
Humic acid complexation with
- Al

As(V)
As(III)
Ca
Co
Cr
Cu
Fe(III)
Hg
Mn
Ni
Pb
Zn

$BaSO_4$ chemistry (revision for high-pressure, high-temperature systems)

$BaSO_4 – H_2O$
$BaSO_4 – NaCl – H_2O$
$BaSO_4 – Na_2SO_4 – H_2O$
$BaSO_4 – KCl – H_2O$
$BaSO_4 – CaCl_2 – H_2O$
$BaSO_4 – CaCl_2$ - $NaCl – H_2O$
$BaSO_4 – MgCl_2 – H_2O$

$CaCO_3$ chemistry (revision for high-pressure, high-temperature systems)

$CaCO_3$ (calcite, aragonite) – $H_2O – CO_2$
$CaCO_3 – NaCl – CO_2$
$CaCO_3 – CaCl_2$
$CaCO_3 – MgCl_2 – CO_2$
$CaCO_3 – Na_2CO_3$
$CaCO_3 – Na_2CO_3 – NaHCO_3$

$FeCO_3$ chemistry (revision)

$FeCO_3 – CO_2 – H_2O$
$FeCO_3 – NaCl – H_2O$
$FeCO_3 – NaClO_4 – H_2O$

Methanol scaling chemistry (revision)

$MgSO_4$ - methanol – H_2O
$MgCl_2$ – methanol – H_2O

Lithium chemistry

Lithium sulfate chemistry

$Li_2SO_4 – NiSO_4 – H_2O$

$Li_2SO_4 – H_2SO_4 – H_2O$
$Li_2SO_4 – MgSO_4 – H_2O$
$Li_2SO_4 – CaSO_4 – H_2O$
$Li_2SO_4 – Na_2SO_4 – K_2SO_4 – H_2O$
$Li_2SO_4 – (NH_4)_2SO_4 – H_2O$

Lithium chloride chemistry

$LiCl – HCl - H_2O$

Lithium sulfate - chloride chemistry

$Li_2SO_4 – LiCl – H_2O$
$LiCl – CaSO_4 – H_2O$
$Li – Mg – SO_4 – Cl – H_2O$

Lithium nitrate chemistry

$LiNO_3 – H_2O$
$LiNO_3 – NaNO_3 – H_2O$
$LiNO_3 – Mg(NO_3)_2 – H_2O$
$LiNO_3 – Ca(NO_3)_2 – H_2O$

Lithium carbonate chemistry

$Li_2CO_3 – Na_2CO_3 - H_2O$
$Li_2CO_3 – LiCl - H_2O$
$Li_2CO_3 – NaCl - H_2O$

Cobalt and cobalt - lithium chemistry

$CoCl_2 – H_2O$
$CoCl_2 - HCl – H_2O$
$CoCl_2 – LiCl – H_2O$
$CoSO_4 – Li_2SO_4 – H_2O$

Uranium chemistry

Uranium (IV) fluoride chemistry

$UF_4 - HF – H_2O$

Uranium (VI) fluoride chemistry

$UF_6 – HF$
$UOF_2 – H_2O$
$UOF_2 – HF – H_2O$

Uranium oxide chemistry

$U_3O_8 – H_2O$ as a function of pH

Iron fluoride chemistry

$FeF_2 – HF$

FeF_3 – HF – H_2O

Aluminum fluoride chemistry

AlF_3 – NH_4F - H_2O including NH_4AlF_4, $(NH_4)_2AlF_5 \cdot H_2O$, $(NH_4)_3AlF_6$

Rare earth chemistry

Rare earth fluorides

LaF_3 – H_2O
CeF_3 – H_2O
NdF_3 – H_2O
NdF_3 – NaF – H_2O
NdF_3 – NH_4F – H_2O
SmF_3 – H_2O
EuF_3 – H_2O
GdF_3 – H_2O
TbF_3 – H_2O
DyF_3 – H_2O
HoF_3 – H_2O
ErF_3 – H_2O
TmF_3 – H_2O
YbF_3 – H_2O
LuF_3 – H_2O

Rare earth phosphates

$GdPO_4$ – H_2O

Rare earth hydroxides

$Gd(OH)_3$ – H_2O

Malonate chemistry

Fe – malonate complexation
Tb – malonate complexation

Acetate chemistry

Fe(III) – acetate complexation

DTPA (diethylenetriaminepentaacetic acid) chemistry

DTPA aqueous speciation
Gd – DTPA complexation
Ca – DTPA complexation

Mg – DTPA complexation

Hydrocarbon chemistry

$C_{80}H_{162}$ (octacontane) – H_2O and generalized interactions
Chemical formulas revised for n-octane and 2,2,4-trimethylpentane

Nitrite chemistry

$NaNO_2$ – H_2O viscosity

Miscellaneous

Solid density revisions:

$2NaOH{\cdot}3Na_2SO_4$
$3CaCl_2{\cdot}H_2O$
$CaCl_2{\cdot}H_2O$
$CaCl_2{\cdot}4H_2O$
$Na_2SO_4{\cdot}5CaSO_4{\cdot}3H_2O$
$Na_2SO_4{\cdot}CaSO_4$
$2Na_2SO_4{\cdot}CaSO_4{\cdot}2H_2O$
$MgCl_2{\cdot}2CaCl_2{\cdot}6H_2O$

Pure liquid density revision:

Melamine

Standard-state entropy revision:

Kr – H_2O

Mackinawite moved to MSEPUB from CRMSE

GEMSE (Geochemical)

Rare earth solids

Rare earth bromides

$LaBr_3$
$CeBr_3$
$PrBr_3$
$NdBr_3$
$SmBr_3$

- $EuBr_3$
- $GdBr_3$
- $TbBr_3$
- $DyBr_3$
- $HoBr_3$
- $TmBr_3$
- $YbBr_3$
- $LuBr_3$

Rare earth iodides

- LaI_3
- CeI_3
- PrI_3
- NdI_3
- SmI_3
- EuI_3
- GdI_3
- TbI_3
- DyI_3
- HoI_3
- ErI_3
- TmI_3
- YbI_3
- LuI_3
- YI_3

Rare earth oxychlorides

- LaOCl
- PrOCl
- NdOCl
- SmOCl
- EuOCl
- GdOCl
- TbOCl
- DyOCl
- HoOCl
- ErOCl
- TmOCl
- YbOCl
- LuOCl
- YOCl

Rare earth molybdates

- $La_2(MoO_4)_3$
- $Pr_2(MoO_4)_3$
- $Nd_2(MoO_4)_3$
- $Sm_2(MoO_4)_3$
- $Gd_2(MoO_4)_3$
- $Dy_2(MoO_4)_3$
- $Ho_2(MoO_4)_3$

$Yb_2(MoO_4)_3$
$Lu_2(MoO_4)_3$
$Y_2(MoO_4)_3$

Rare earth sulfides

La_2S_3
Ce_2S_3
Nd_2S_3

Rare earth anhydrous sulfates

$Ce_2(SO_4)_3$
$Nd_2(SO_4)_3$

MSE-SRK model

Hydrocarbon chemistry

$C_{80}H_{162}$ (octacontane) – H_2O and generalized interactions
Chemical formulas revised for n-octane and 2,2,4-trimethylpentane

AQ model

Miscellaneous

Solid density revisions:

$2NaOH \cdot 3Na_2SO_4$
$3CaCl_2 \cdot H_2O$
$CaCl_2 \cdot H_2O$
$CaCl_2 \cdot 4H_2O$
$Na_2SO_4 \cdot 5CaSO_4 \cdot 3H_2O$
$Na_2SO_4 \cdot CaSO_4$
$2Na_2SO_4 \cdot CaSO_4 \cdot 2H_2O$
$MgCl_2 \cdot 2CaCl_2 \cdot 6H_2O$
$B(OH)_3$

Standard-state entropy revision:

Kr – H_2O

Chemical formulas revised for n-octane, 2,2,4-trimethylpentane, and $UO_2(AsO_4)_2$

Name fixed for magnetite

CORROSION KINETICS:

Alloy 22 – revision

Corrosive environments:

NaCl
Seawater – O_2
H_2S – NaCl
CO_2 – NaCl
CO_2 – H_2S – NaCl
NaOH
Formic acid
H_2SO_4
HCl
HNO_3
H_3PO_4
HCl – H_2SO_4
HCl – HNO_3
HF
HF – H_2SO_4
H_2SO_4 – HNO_3
HF – HNO_3
$FeCl_3$ – $FeCl_2$ – NaCl – HCl
Na_2SO_4 – $NaNO_3$ – H_2SO_4 – O_2
$CuCl_2$ – CuCl – NaCl – HCl
LiCl

Repassivation potential parameters:

Cl^-
H_2S
$SO4^{2-}$
NO_3^-
OH^-
$VO4^{3-}$
MoO_4^{2-}

Alloy 276 – revision

Corrosive environments:

NaCl
Seawater – O_2
H_2S – NaCl
CO_2 – NaCl
CO_2 – H_2S – NaCl
NaOH
Formic acid
Acetic acid
Acetic acid – Formic acid
H_2SO_4
HCl
HCl – O_2

HNO_3
H_3PO_4
H_3PO_4 – NaCl – O_2
HCl – H_2SO_4
HCl – HNO_3
HF
HF – H_2SO_4
H_2SO_4 – HNO_3
HF – HNO_3
$FeCl_3$
$FeCl_3$ – $FeCl_2$ – NaCl – HCl
$FeCl_3$ – HCl
$FeCl_3$ – H_2SO_4
$CuCl_2$ – CuCl – NaCl – HCl
$CuCl_2$ – H_2SO_4
LiCl
CrO_3
$AlCl_3$

Repassivation potential parameters:

Cl^-
H_2S
$SO4^{2-}$
NO_3^-
OH^-
$VO4^{3-}$
MoO_4^{2-}

Alloy 625 – revision

Corrosive environments:

NaCl
Seawater – O_2
H_2S – NaCl
CO_2 – NaCl
CO_2 – H_2S – NaCl
NaOH
Formic acid
Acetic acid
Butyric acid
H_2SO_4
HCl
HNO_3
H_3PO_4
HCl – H_2SO_4
HCl – HNO_3

HF
$H_2SO_4 – HNO_3$
$HF – HNO_3$
$FeCl_3$
$FeCl_3 – NaCl$
$FeCl_3 – FeCl_2 – NaCl – HCl$
$CuCl_2 – CuCl – NaCl – HCl$
$NaNO_3 – O_2$
$Na_3VO_4 – O_2$
$Pd_2SO_4 – O_2$

Repassivation potential parameters:

Cl^-
H_2S
$SO4^{2-}$
NO_3^-
OH^-
$VO4^{3-}$
MoO_4^{2-}

Alloy 825 – revision

Corrosive environments:

NaCl
Seawater – O_2
$H_2S – NaCl$
$CO_2 – NaCl$
$CO_2 – H_2S – NaCl$
NaOH
$NaOH – O_2$
Formic acid
Acetic acid
Butyric acid
H_2SO_4
HCl
HNO_3
H_3PO_4
$H_3PO_4 – HF$
$H_3PO_4 – HF – O_2$
$NaCl – H_2SO_4$
$HCl – HNO_3 – O_2$
HF
$HF – HNO_3$
$FeCl_3$
$FeCl_3 – HCl$
$FeCl_3 – FeCl_2 – NaCl – HCl$

$CuCl_2$ – CuCl – NaCl – HCl

Repassivation potential parameters:

Cl^-
H_2S
$SO4^{2-}$
NO_3^-
OH^-
$VO4^{3-}$
MoO_4^{2-}

Alloy 2205 – revision

Corrosive environments:

NaCl
Seawater – O_2
H_2S – NaCl
CO_2 – NaCl
CO_2 – H_2S – NaCl
NaOH
$CaCl_2$
Formic acid
Acetic acid
H_2SO_4
HCl
H_2SO_4 – HCl
HNO_3
H_3PO_4
H_2SO_4 – HNO_3
H_2SO_4 – H_3PO_4
H_3PO_4 – HF
H_2SO_4 – H_3PO_4 – HF
H_3PO_4 – HNO_3
HNO_3 – H_2SiF_6
HNO_3 – H_3PO_4 – HF
HNO_3 – H_2SiF_6 – H_3PO_4
HF – HNO_3
$FeCl_3$
$FeCl_3$ – HCl
$FeCl_3$ – $FeCl_2$ – NaCl – HCl
$CuCl_2$ – CuCl – NaCl – HCl

Repassivation potential parameters:

Cl^-
H_2S
$SO4^{2-}$
NO_3^-

OH^-
$VO4^{3-}$
MoO_4^{2-}

Alloy 2550

Corrosive environments:

NaCl
Seawater – O_2
H_2S – NaCl
H_2S – NaCl – Acetic acid
CO_2 – NaCl
CO_2 – NaCl – Acetic acid
CO_2 – H_2S – NaCl
CO_2 – H_2S – NaCl – Acetic acid
Formic acid
Acetic acid
HCl

Repassivation potential parameters:

Cl^-
H_2S
$SO4^{2-}$
NO_3^-
OH^-
$VO4^{3-}$
MoO_4^{2-}

Alloy S13Cr

Corrosive environments:

NaCl
NaCl – $NaHCO_3$
Seawater – O_2
H_2S – NaCl
H_2S – NaCl – Acetic acid
CO_2 – NaCl
CO_2 –Seawater – O_2
H_2S – NaCl – NaAcetate
CO_2 – NaCl – Acetic acid
$CaCl_2$ – CO_2 – Acetic acid
CO_2 – H_2S – NaCl – Acetic acid – NaAcetate
CO_2 – H_2S – NaCl
HCl

H_2SO_4
CsFo – KFo
$KCOOH – K_2CO_3 – KHCO_3 – CO_2$

Repassivation potential parameters:

Cl^-
H_2S
$SO4^{2-}$
NO_3^-
OH^-
$VO4^{3-}$
MoO_4^{2-}

Alloy S15Cr

Corrosive environments:

NaCl
Seawater
$H_2S – NaCl$
$CO_2 – NaCl$
$CO_2 – H_2S – NaCl – Acetic\ acid$
$CO_2 – H_2S – NaCl$
HCl

Repassivation potential parameters:

Cl^-
H_2S
$SO4^{2-}$
NO_3^-
OH^-
$VO4^{3-}$
MoO_4^{2-}

Alloy S17Cr

Corrosive environments:

NaCl
$Seawater – O_2$
$H_2S – NaCl$
$CO_2 – NaCl$
$CO_2 – H_2S – NaCl – Acetic\ acid$
$CO_2 – H_2S – NaCl$
HCl
Formic acid

Formic acid – O_2

Repassivation potential parameters:

Cl^-
H_2S
$SO4^{2-}$
NO_3^-
OH^-
$VO4^{3-}$
MoO_4^{2-}

Alloy 2507 – revision

Corrosive environments:

Acetic acid

Butyric acid

H_2CO_3

$CO_2 – H_2S – NaCl$

$H_2S – NaCl –$ Acetic acid

$CO_2 – H_2S – NaCl –$ Acetic acid

Alloy 28 – revision

Corrosive environments:

Butyric acid

H_2CO_3

$CO_2 – H_2S – NaCl$

Alloy 29 – revision

Corrosive environments:

Butyric acid

H_2CO_3

$CO_2 – H_2S – NaCl$

Alloy 2535 – revision

Corrosive environments:

Butyric acid

H_2CO_3

$CO_2 – H_2S – NaCl$

Engine/Solver - Features

Bug ID	AREA	Problem	Resolution
94	Engine	**Add support for pH calculations at a reference temperature**	Typically, the reference temperature is 25°C.
259	All Products	**Revulytics data collection is removed from all products**	This feature did not provide enough value to OLI and was a problem for some governmental agencies. It has been disabled but still exists in older products.
750	Solver	**Enhanced CO2 dominated REDOX calculations**	These calculations sometimes did not converge.
1036	Engine	**Add a hardness calculation for water samples**	Calculation type added.
1242	Solver	**Create a linear solver to break apart ions back into user supplied inflows for Water Analysis and OLI Flowsheet**	Engine work developed to support this feature.
1316	Engine	**Total Inorganic Carbon implemented for alkalinity**	Engine work to support TIC calculations
1320	Engine	**Added support for direct stream adjustment**	Instead of using a Manipulator Block, the inlet stream can be directly adjusted via controller.
1444	Engine	**Virtual streams implemented**	Engine work to allow virtual streams
1545	Solver	**RO membrane speedup**	Decreased calculation time for RO membranes
1881	Solver	**RO membrane speed up – edge cases**	Detected marginal cases and protected from crashes.

Engine/Solver - Bugs

Bug ID	AREA	Problem	Resolution
1265	Solver	**Unconverged cases in MSE-SRK, these should converge easily.** **In this case it is a temperature survey at low pressure. There are some intermediate unconverged points which make no sense since high ranged points do converge**	The vapor results over water boiling point are all invalid. MSE-SRK has issue to calculate only organics with solids because there's no ions in the 2nd liquid phase. The engine pushes all organic species to vapor phase and report converged. There will be a story to trap out and fail the L2-S calculation in MSE-SRK and suggest using MSE.
1273	Solver	**MSE-SRK case tripped sublimation code and formed ICE at temperature above 0°C.**	There's a line to remove water sublimation in subleqn.for, which is currently commented out. When this line is taken in, the bug is solved. Test cases will be run to confirm it.
1307	Solver	**A simple mixer-reactor is converting Mg(OH)2 to the surface species. It works at very low conversions and high conversions, but at 0.1 it fails. The settings are at 0.1 so that you can see the NAN in the output. Then there is a sensitivity that goes from 0.01 to 0.5, and it appears to work seamlessly.**	Added a phase check in the AQ model initializer.
1308	Solver	**$(NH_4)_2SO_4$ Sublimation at lower temperatures and in presence of N_2 fails to predict the solid phase**	Tightened the tolerance in the norm calculation for sublimation calculation.
2229	Engine	**Memory usage grows each time you run a case in Flowsheet**	Memory leak found and plugged

OLI Studio/Analyzer - Features

Bug ID	AREA	Problem	Resolution
61	Water Analysis	**A customer is requesting that entry of their lab data be made easier, ex: they have Total Phosphate right now they have to pick an ionic species and calculate the correct amount based on the data they have, the UI should be able to help them out on this.**	User can enter total "P" in the water analysis grid and provide a concentration number in mg/L. The number will be applied to the underlying P(+5) species, and later converted to moles of PO4 ion during calculation.
79	Reports/Plots	**Solids that are out of TRANGE are not displayed by default**	The user can decide to plot species out of TRANGE.
398	UI	**Single Point volume reconcile added for concentration units**	This was implemented previously for surveys but is now available for single point calculations.
437	Reports	**Dissolved CO_2 has now been parsed out from HCO_3^{-1} values in brine totals.**	Previously in the report, CO_2 was incorrectly combined with HCO_3^-
563	Calculation	**TDS now has an option for Rigorous or Estimated TDS**	
1183	Units Manager	**Hardness is a new calculation type. The units need to be "mg/L of Mg^{+2} and Ca^{+2}"**	Units added
1328	Set Up	**A first "First Run Wizard" has been added to set up initial conditions for the program.**	The user can now initially set up units, file locations among others the first time the program is run.
1332	File Manager	**Saving files as a template**	User can save a case as template (*.oat). After opening a template file, it will automatically be marked as modified and (oat) is removed from the file name.
1452	Set Up	**Allow user to select units set associated with an object in First Run Wizard**	This extends the feature in #1328 to target an object.

1749	Data Collection	**OLI no longer supports the Revulyitics data collection program. The opt-in/out dialogs need to be removed**	Dialogs removed
1808	Database	The new data system no longer needs the old ESP format databases. The import tool is no longer needed, and the button should be removed from the dialog	Button removed.

OLI Studio/Analyzer - Bugs

Bug ID	AREA	Problem	Resolution
266	ScaleChem	**Related to #360**	
360	ScaleChem	**Facilities design tab is slow to refresh with a large number of nodes**	Optimized the refresh algorithms.
401	OLI Studio	**Closing the file while calculating causes a crash**	The code now asks the user if they would like to cancel the calculations, if they do it then cancels the calculations and informs them to try saving again. Trying to directly complete the task led to other crashes due to timing. To fix this way will take too much time as I do not think this is encountered to often.
633	Stream Analyzer	**No sublimation solids when expected**	The engine was updated to use new tolerances for the appearance of a sublimation phase.
926	Stream Analyzer	**The *Template Manager* for Water Analysis allows the user to save a roster of species that they feel are more useful than the templates supplied with OLI Studio.** **If one of the species is removed from the standard list and saved as a new template and then that template is used, the standard species are still there. It is like the standard template will overlay any existing template. Templates with more than the standard species work.**	Templates that contain no species were not being applied, updated code to apply empty/blank templates.
1305	Stream Analyzer	**When the survey is created from a stream using conc units, the density correlation should have been set to Parent condition. It is appearing as Fixed condition when I do it. Fixed condition creates the precise problem we wanted to avoid when creating this function. Please confirm that Parent condition is the default setting.**	Reset default to parent stream condition.
1377	ScaleChem	**Scale Object has multiple whole fluid entries when it should have only 1**	UI cleaned up to show only a single whole fluid.
1540	Stream Analyzer	**The attached case has two single point calculations. The first is marked with No H2O. This does not mass balance the F(-1) material balance group. It is off in the ppm range (mole basis). Also, it is reporting an aqueous phase (liquid 1) when there is no H2O present.** **The other case marked w/ H2O properly converges, has a proper mass-balance and does not have a Liquid 1 phase.**	This case should result in two liquid phases even with small amount of water added in. The current engine has a threshold when water inflow is less than 1e-7 mole fraction to turn off 2nd liquid option. The threshold in modified to 1e-10 to allow more accurate prediction for such case. For the charge balance issue, there are two reactions affecting HF dissociations: Eq1: H2FION + FION = 2HFAQ Eq2: HFAQ + H2O = H3OION + FION In our solver, H2O is always participating even though there is no inflow, that means Eq2 is allowed during the calculation. However, existing of H2O and H3OION increases the residual of H2O mass balance, which means H2O and H3OION are removed eventually. But it will not revert Eq2, therefore it results in slight charge unbalance. This cannot be solved now because H2O is always treated as a free variable now.
1541	ScaleChem	**Brine reconcile has negative values for ion concentrations**	The file was corrupted because of a bad density value. Code was placed to prevent a negative density. See #1700
1700	Stream Analyzer	**The brine in the case "Brine" is corrupted. There is an error message about zero flows. It seems to have taken the Na+ ion and made it very negative.**	Debugged case and found total volume was negative, not sure how it went negative. Added code during case load to identify the negative volume and reset it.

1745	ScaleChem	**A block has a total mass of 119,000 Kg/day entering. The report only has 3000 Kg/Day being reported.**	An error in the MBG types had occurred. Some species being converted from "True" species to MBG were lost.
1797	Stream Analyzer	**Water Analysis now shows volume reconcile options which it should not.**	This was trapped out in the code and prevented
1960	ScaleChem	**Misspellings in brine report detected**	Misspellings are corrected.
2002	ScaleChem	**Cations not being reported in Brine report**	Ions added back in (found in beta testing)
2014	ScaleChem	**Calculation not done message when Calculation is succeeded: Brine Analysis**	Removed errant message
2018	OLI Studio	**Plot legend disappears when moved.**	The underlying controls (Stingray) were updated but not merged properly.
2032	Stream Analyzer	**0 deg C point shows a blank line in the report**	Report is now properly managed.
2079	Stream Analyzer	**Water Analysis Template does not understand about aggregate species such as Total P**	Aggregate species added to the template.
2094	Stream Analyzer	**Solid phase enthalpy may exist when there is no solid phase**	If solid mass is 0 but solid enthalpy is not, check if surface exists. If so, unhide the nonzero solid enthalpy.

OLI Flowsheet: ESP / ESP-FS - Features

Bug ID	AREA	Problem	Resolution
57	Model Generation	**Include the same component search features as in OLI Studio**	Both programs now use the same UI.
300	UI	**The permeate and concentration lines from a RO membrane are now shaded**	In previous versions, the lines were indistinguishable making it difficult to read the PFD.
437	Reports	**Dissolved CO_2 has now been parsed out from HCO_3^{-1} values in brine totals.**	Previously in the report, CO_2 was incorrectly combined with HCO_3^-
503	File Management	**Added an RO membrane example to the installation set**	Membrane example added.
519	Model Generations	**The ability to use older installed master databases was implemented**	During Q/A work, it is necessary to test the new program with older, vetted databases.
532	UI	**Component efficiencies were added to multi-stage unit operations**	This was missed in previous versions of the software although present in ESP-Original.
535	UI	**The outlets for each block now support a drop-down box to see other streams for connection**	This allows blocks to be easily added upstream of existing blocks.
550	UI	**A controller cannot directly adjust an inlet stream.**	Manipulator Blocks are no longer required.
552	UI	**Multiple image support for unit operation images now supported**	Mixers can be changed into Autoclaves by a right-click.
828	UI	**Added the ability to enter ionic input (similar to Water Analyzer) instead of a copy/paste feature**	The standard Water Analysis functionality is now included in OLI Flowsheet.
1046	UI	**RO membranes use NACL as part of the manufacturer specifications. The component should automatically be added when using RO membranes**	NaCl is automatically added to the chemistry model if present in the specification data.
1060	Engine	**In this case, a pump is used near the beginning of the process. Cp is enabled but all the streams downstream of the pump have the Cp value set to zero.** **If you replace the pump with a mixer the Cp values are reported.**	The pump uses EQSOLVED for flash calculations. prior to the call it updates the property calculation vector IDEFNA. This is overwritten with 0 for the said properties with the current strategy. passing NIPROP = 0 solves the issue.
1209	UI	**Add isochoric calculations to the separator block**	Added option
1227	Calculations	**A pH can now be calculated at a reference temperature in addition to stream conditions**	Users frequently reference a pH at 25°C. This allows the direct reporting of this value without needed any additional calculation steps.
1322	UI	**A feedback controller, when the target of a feed forward controller needs a default action of "Calculate After Block" to be added.**	The option has been added. This cleans up the block order code and makes for more stable calculations.
1328	Set Up	**A first "First Run Wizard" has been added to set up initial conditions for the program.**	The user can now initially set up units, file locations among others the first time the program is run.
1329	UI	**Isochoric calculations added to separator unit operations**	This makes the mixer and separator unit operations consistent.

1332	File Management	**A process file can now be saved as a template**	EST file types created. When saved for the first time the file becomes the standard ESP file type.
1413	UI	**Virtual Stream: Block re-order algorithm implemented**	The addition of virtual streams has required that the block-order program be enhanced to cross between disconnected flowsheets.
2035	UI	**If the process is changed, no "*" appears in the title bar.**	"*" if the process has changed.
2092	Model Generation	**Flowsheet does not regenerate the chemistry model(s) if no changes in chemistry are detected**	This will speed up the process by not automatically generating the internal model each time the program runs. The generation only occurs if a change in chemistry is detected.

OLI Flowsheet: ESP / ESP-FS - Bug

Bug ID	AREA	Problem	Resolution
335	Sensitivity	**Error in data storage for an Analysis calculation**	This case had 58,564 points. This was too much. The error message has been modified to suggest reducing sensitivity analysis calculation points.
632	UI	**Restarting a TEAR stream fails when surface complexation species are in the model (CPM type)**	There was a bug in the Flowsheet: ESP application-layer code due to which certain dynamically created surface complexation species were not properly characterized during model build. This was causing errors in obtaining mol-wt of said species and affected the logic that split the composition of solid phases reported by the engine into the real solid phases and surface species.
668	Report	**Multistage unit operations do not report surface tension as a variable even though the optional parameter was enabled.**	The check to determine if surface tension was stored in a stream's results was incorrect. Fixed the check.
915	Engine	**Unconverged case - RO Membrane with high hydraulic pressure does not converge**	From DOW: The maximum recommended pressure drop across a single element is 15 psid (1bar) or 50 psid (3.5 bar) across multiple elements in a pressure vessel, whichever value is more limiting. We recommend designing at maximum of 80% (12 psid) for any element in a system. An article from DOW has been added as reference. Pressure drop could be much higher if not operated according to the recommendation from the manufacturer. In case pressure drop in the concentrate side goes out of bound as described above, few checks were added to limit the allowed pressure drop in the concentrate side.
925	Engine	**CSplit is creating mass in a calculation. Material balance groups were used to define the split fractions**	This feature was never properly implemented in the engine. This has been disabled for V10.0.0
950	Engine	**RO case is stuck in initialization**	The issue was cross-referencing NACL from K-coefficients. Test species was 'NACL' which is a solid, but the solid phase was turned off. Since there were no K-coefficients for NACL, it could not map permeability for other cations/anions. This has been fixed.
1030	Model Generation	**Very long times for model generation with multiple models.**	Model generation time was sped up by 10X
1031	UI	**Block order not properly ordered with feed forward controllers**	The targeted controller is now forced to execute after the feed forward controller.
1060	UI	**A pump wipes out transport properties downstream of the unit.**	The pump uses EQSOLVED for flash calculations. prior to the call it updates the property calculation vector IDEFNA. This is overwritten with 0 for the said properties with the current strategy. passing NIPROP = 0 solves the issue.
1147	Engine	**Suez brand membrane AE-400 with high TDS calculated a negative flux. The Osmotic pressure was lower than the hydraulic pressure.**	This is not really an RO membrane but a NF membrane.
1272	UI	**Streams with blank names (to hide them) crashed the program**	Blank stream names are trapped and not allowed.
1307	Report	**NaN (not-a-number) values are reported in the output (REACTOR)**	Added a phase check in the AQ model initializer
1378	UI	**Insufficient virtual memory in large cases**	This is a large system. It can be completed using memory ~400 Mb during the calculation. There is large amounts of memory used in flowsheet UI to identify the block order. The block order identification was optimized.
1418	Report	**Flowsheet shows different apparent and true moles for organic species in MSE-SRK and AQ. There are input**	When stream total flow is by volume, the stream is calculated with a given mole flow with fixed T and P. Then,

		streams only contains organic species (CH4 and C10h22). When the stream total flow is by volume, results show that total true moles and total apparent moles are different. When water is added, the problem is resolved. When the stream total flow is by mole, it doesn't have problem.	comparing the calculated volume to the input volume, the total vapor, aqueous, and organic mole flows are multiplied by the ratio. In strfact.for where the ratio is applied, there's a typo that copying total organic moles in EVEC from a wrong value. Therefore, total true moles (from EVEC) miss the 2nd liquid part but total apparent moles (from GVEC) is correct.
1768	Model Generation	**Changing a pseudocomponent name changed the results**	The internal order of species was not updated with the name change. Thus, the wrong values were passed.
1975	UI	**The name change symbol in the right-click menu is confusing.**	Changed to "Change Icon"
1851	UI	**Bad callout for a block with a turbine**	Call out updated with proper turbine values.
1920	UI	**Removing "The flowsheet is fragmented" message for Fragmented flowsheet**	Fragmented flowsheets are now allowed.
2058	UI	**Cannot change color of added text box**	Color options implemented
2182	UI	**Periodic Table Search Option Incorrect in OLI Flowsheet and OLI Databook. The search option "Any of selected" and "All of selected" are acting opposite to what is should do. This bug exists in both Flowsheet and Databook. However, in OLI Studio it behaves correctly.**	Search algorithm updated
2226	Solver	**Mass-balance errors detected when using volumetric units**	Volume reconciles were not properly accounted in the solver.
2228	Solver	**When total stream amount is specified in volume, calculated Liquid-2 true species total moles value is not correct (Related to case 2226)**	Volume reconciles were not properly accounted in the solver.

Alliance Products - Features

Bug ID	Program	Problem	Resolution
1552	Aspen Plus, Hysys	**32 and 64 bit supported via a compiler update**	Aspen V11 is 64 bit only, OLI needs to have a 64 bit version. The 32 bit is for older versions of Aspen.

Alliance Products - Bugs

Bug ID	Program	Problem	Resolution
490	Aspen Hysys	When running the attached case in V10 or V11 of HYSYS the single stream does not converge, there is also an OLI Studio file attached with the same stream. This case also fails unless the guess temperature is raised closer to the result temperature which is around 81C.	The Liquid Guess in the initializer for Fix Vapor Fraction/Free T can sometime be below the limit of sensitivity to the residuals. This results in very slow convergence, in this case. This value has been increased to allow for rapid convergence.
1025	Aspen Plus / Chemistry Wizard	**The generated BKP file creates the same K-SALT coefficients for all solids in MSE. They are different in the AQ framework. This might give RADFRAC bad initial guesses.**	When using AQ model, solid K values are generated from K-fit parameters. Both in polynomial forms, we convert the K-fit coefficients to K-salt coefficients and reported in the ASPEN bkp file. However, in MSE, HKF is used to calculate K values and we just report dummy K-salt values in ASPEN bkp file. Even though the solver correctly calculation the solubility, the dummy K-salt coefficients might be used as bad initial guesses for other calculations like RADFRAC, as Jim mentioned. The same situation applies to K-equilibrium and PLXANT in ASPEN. For CPIG, ASPEN default parameters are used if the component has ASPEN component name (ASNM) in OLI databank. Otherwise, dummy values are reported. We need to: 1. identify which dummy properties ASPEN will use rather than calling OLI-Engine; 2. if we need to correctly report those parameters, we have to implement a method to regress our properties with ASPEN's polynomial coefficients.
1182	Aspen Plus / Chemistry Wizard	**The Chem Wiz for Aspen Plus does to write the alias ID to the BKP file. In the attached files, the CWA has an alias of P4O10 which I entered. It should be in the BKP file, but it is not.**	Bug in code caused the alias name not to compared inflow species * The comparison was done with species name * This will happen only if there is no ASNM value for solid chapter for the species * Fixed up updating code to the correct check
1647	Aspen Plus	**A file converges the base case but fails the analysis case.**	In this case, user called a bubble point calculation by fixing P and vapor amount to calculate T. An initial guess for T is

		What i did was to run several base cases over the range of the values in the Analysis case. All converge. This indicates to me that the base interface is working correctly. **The analysis cases fail with the Aspen Error in Aspen Plus V10** **** ERROR WHILE GENERATING PROP-TABLE: "MIX-1" (OFLASH.1)** **Error: Electrolyte equilibrium failed to converge.**	need, where we have one-line code to estimate based on the pressure. However, it uses the pressure from the stream vector passed in rather than calling an ASPEN routine to get the user provided pressure. In ASPEN flowsheet block calculation, the pressure in the stream vector is from the input stream (different to the block setting). But it can still provide a reasonable initial guess T. However, in ASPEN analysis, the pressure in stream vector was uninitialized (1e35) which resulted in bad initial guess T (less than -300 C) which crashed our solver. The initial guess T is changed to be estimated from the pressure get from ASPEN interface, which solved the problem.
1757	Aspen Plus	**DHFORM value in BKP file is incorrect when passed from OLI to Aspen Plus**	Encoding code corrupted the values for HKF and thus created a bad value.

OLI Developer Edition - General

Bug ID	Program	Problem	Resolution
2170	Engine	The attached vb.net solution causes an access violation when calling EQLABAN	Access violation when the number of inflows exceeded number of species. This was corrected.

OLI Framework - General

Bug ID	Program	Problem	Resolution
1925	Security	License Manager should auto enable logging of users. With 3.4.3 this feature is turned off. It should also auto roll over each month.	Auto Enable turned on.
2153	Error Messaging System	Add full version to about dialog ex: 10.0.1.14.	Full version added
2243	Security	If OLI Flowsheet is started and the license server is not available, the program will crash after the error message is displayed.	Security layer updated to protect against the crash