

Summary of Terms

Duration

The project will be carried out over a 3-year and 9-month period (4/1/2009 – 12/31/2012).

Deliverables

The possible deliverables for this project have been outlined under the Objectives above. With sufficient support it is our hope to accomplish all of these objectives within the duration of the project. However, this will be largely dependent upon the number of subscribers to this consortium.

The actual schedule and timing of deliverables will be strongly dependent upon the priorities expressed by the member companies. Thus, if a member company sets a particular chemical system as its first priority, that system will be given high priority for development.

Benefits

Consortium members would receive a number of unique benefits based upon their participation. The benefits include:

- Allowing OLI to accomplish the objectives listed above, which can be used to great benefit by the individual members.
- The assurance that each member, in conjunction with item 3 of the objectives listed above, will be able to prioritize up to 25 workdays of OLI's thermophysical modeling services based upon such work going to the OLI public databank. Alternatively, if the work is to be proprietary (based at least partially on client data), then up to 12.5 workdays could be provided. This represents \$25,000 of modeling services fees that will be provided to each member.
- Providing to each member, periodically, comprehensive Excel spreadsheet documentation containing the quality assurance material comprised of experimental data, literature citations, and comparative plots. Only members of the MSE Consortium will be provided the full content of these spreadsheets covering the MSE Public Databank.
- Providing data fitting software utilized in conjunction with MSE together with an expert user training course in how best to utilize these facilities. Data fitting is a highly complex task that requires a thorough understanding of both thermodynamic properties and the model. For electrolyte systems, regressions are usually dramatically more involved than for nonelectrolytes. Tremendous progress has been made in the OLI fitting procedures with the introduction of multiproperty regressions and elimination of empirical fitting functions (a.k.a. Kfits) in favor of rigorous adjustment of thermochemical properties. There are already some "power users" outside of OLI who can effectively use the regression tool. We are offering to train members of the consortium in the use of the regression program so that they can become proficient in their own regressions.

- Earliest possible access to the software that results from this work. This can make all the difference on a time-critical application.
- Technical steering of the project, which will assure that the needs of individual member companies are reflected in this work. This provides your company with assurance of monitoring the project and working with other companies as well.
- Leveraging funding from any additional sponsored research or professional projects, which are directed towards the objectives of this project.
- Leveraging industry support for this Consortium based upon the participation and support of other members. The result is that funds from your company are multiplied.

Commitment

OLI is seeking a commitment of \$25,000/year for each of three years to cover fully the cost of membership. This sum can be paid in three installments of \$25,000 each, due on 1/1/2010, 1/1/2011, and 1/1/2012.

OLI has extended the period of open membership from 4/01/2009 until 12/31/2009.

We appreciate your interest in this proposal and look forward to the possibility of working with your company in conjunction with this exciting project.

Appendix 1: Chemistry Covered in MSE III

1. Binary and principal ternary systems composed of the following primary ions and their hydrolyzed forms:

Cations: Na^+ , K^+ , Mg^{2+} , Ca^{2+} , Al^{3+} , NH_4^+

Anions: Cl^- , F^- , NO_3^- , CO_3^{2-} , SO_4^{2-} , PO_4^{3-} , OH^-

2. Multicomponent Na salts

Na^+ - F^- - NO_3^- - NO_2^- - CO_3^{2-} - SO_4^{2-} - OH^-

3. Li chemistry

Li^+ - K^+ - Mg^{2+} - Ca^{2+} - Cl^-

4. Ba chemistry

Ba^{2+} - Cl^- - CO_3^{2-} - SO_4^{2-} - OH^- - BO_2^- - Na^+ - K^+ - Mg^{2+} - Ca^{2+}

5. Borate chemistry

H^+ - Li^+ - Na^+ - Mg^{2+} - Ca^{2+} - BO_2^- - OH^-

H^+ - Li^+ - Na^+ - BO_2^- - HCOO^- - CH_3COO^- - Cl^- - OH^-

6. Aqueous acids, associated acid oxides and acid-dominated mixtures

H_2SO_4 - SO_3

HNO_3 - N_2O_5

HNO_2

H_3PO_4 - $\text{H}_4\text{P}_2\text{O}_7$ - $\text{H}_5\text{P}_3\text{O}_{10}$ - P_2O_5

H_3PO_2

H_3PO_3

HF

HCl

HBr

HI

H_3BO_3

$\text{CH}_3\text{SO}_3\text{H}$

$\text{NH}_2\text{SO}_3\text{H}$

HFSO_3 - HF - H_2SO_4

HI - I_2 - H_2SO_4

HNO_3 - H_2SO_4 - SO_3

H_3PO_4 with various calcium phosphates

H^+ - Na^+ - Cl^- - NO_3^-

H^+ - Na^+ - Cl^- - F^-

H^+ - Na^+ - PO_4^- - OH^-

H^+ - NH_3 - NO_3^- - SO_4^{2-}

H^+ - NH_3 - Cl^-

7. Sulfide and H_2S chemistry (other than transition metals)

NH_4HS - H_2S - NH_3

H_2S - H^+ - Na^+ - Cl^-

Na_2S - NaHS - H_2S

8. Inorganic gases in aqueous systems

CO₂ - NH₃ - H₂S
SO₂ - H₂SO₄
N₂
O₂
H₂ - H⁺ - Na⁺ - Cl⁻

9. Silica chemistry

Si^{IV} - H⁺ - OH⁻ - Na⁺

10. Hydrogen peroxide chemistry

H₂O₂ - H₂O - H - Na - OH - SO₄ - NO₃

11. Transition metal aqueous systems

Fe^{II} - H⁺ - OH⁻ - Cl⁻ - Br⁻ - SO₄²⁻ - NO₃⁻ - S²⁻ - Ac⁻ - NH₃ - NH₄⁺ - Na⁺
Fe^{II} - Cr^{III} - H⁺ - OH⁻
Fe^{III} - H⁺ - Cl⁻ - SO₄²⁻ - NO₃⁻
Ni^{II} - H⁺ - OH⁻ - Cl⁻ - SO₄²⁻ - NO₃⁻ - PO₄³⁻ - S²⁻ - NH₃ - Na⁺ - morpholine
Ni^{II} - Cr^{III} - H⁺ - OH⁻
Ni^{II} - Ti^{IV} - H⁺ - OH⁻
Ni^{II} - Fe^{II} - H⁺ - OH⁻ - BO₂⁻
Cr^{III} - H⁺ - OH⁻ - Cl⁻ - SO₄²⁻ - NO₃⁻
Cr^{VI} - H⁺ - OH⁻ - NO₃⁻
Mo^{III} - H⁺ - Cl⁻ - OH⁻ - H₂
Mo^{IV} - H⁺ - Cl⁻ - OH⁻ - H₂
Mo^{VI} - H⁺ - OH⁻ - Cl⁻ - SO₄²⁻ - NO₃⁻
W^{VI} - H⁺ - OH⁻ - Na⁺ - Cl⁻, NO₃⁻
W^{IV} - H⁺ - OH⁻
Sn^{II} - H⁺ - OH⁻ - CH₃SO₃⁻
Sn^{IV} - H⁺ - OH⁻ - Cl⁻
Zn^{II} - H⁺ - Cl⁻ - SO₄²⁻ - NO₃⁻
Zn^{II} - Li⁺ - Cl⁻
Cu^{II} - H⁺ - OH⁻ - Cl⁻ - SO₄²⁻ - NO₃⁻ - H₂S - S²⁻ - CO₂ - CO₃⁻ - NH₃ - Na⁺ - morpholine - Et₂NH
Cu^I - H₂S - S²⁻
Cu^{II} - Cu^I - Fe^{II} - Fe^{III} - H⁺ - OH⁻ - S²⁻
Ti^{IV} - H⁺ - OH⁻ - Ba²⁺ - Cl⁻ - OH⁻ - BuO⁻ - Na⁺
Pb^{II} - H⁺ - OH⁻ - Na⁺ - Cl⁻ - SO₄²⁻ - S²⁻ - H₂S - CO₃²⁻ - ClO₄⁻ - K⁺ - Si⁴⁺
Pb^{II} - Ti^{IV} - H⁺ - OH⁻
Pb^{IV} - H⁺ - OH⁻

12. Miscellaneous inorganic systems in water

NH₂OH
Na₂S₂O₃
Na⁺ - BH₄⁻ - OH⁻
Na⁺ - SO₃²⁻ - SO₂ - OH⁻
HCN - NaCN

13. Most elements from the periodic table in their elemental form

14. Base ions and hydrolyzed forms for the majority of elements from the periodic table

15. Organic acids/salts in water and alcohols

Formic

H^+ - Li^+ - Na^+ - Formate - OH^-

Formic acid – MeOH - EtOH

Acetic

H^+ - Li^+ - Na^+ - K^+ - Ca^{2+} - Ba^{2+} - Acetate - OH^-

Acetic acid – MeOH – EtOH – CO_2

Citric

H^+ - Na^+ - Citrate - OH^-

Oxalic

H^+ - Oxalate – Cl^- - SO_4^{2-} , NO_3^- , MeOH, EtOH, 1-PrOH

Malic

Glycolic

Acrylic

Adipic

H^+ - Na^+ - Adipate

Adipic acid – MeOH, EtOH

Nicotinic

H^+ - Na^+ - Nicotinate

Nicotinic acid - EtOH

Terephthalic

H^+ - Na^+ - Terephthalate

Terephthalic acid – MeOH, EtOH

Isophthalic

Isophthalic acid - EtOH

Trimellitic

Trimellitic acid - EtOH

16. Hydrocarbon systems

Hydrocarbon + H_2O systems

Straight chain alkanes: C1 through C30

Isomeric alkanes: isobutane, isopentane, neopentane

Alkenes: ethene, propene, 1-butene, 2-butene, 2-methylpropene

Aromatics: benzene, toluene, o-, m-, p-xylenes, ethylbenzene, cumene, naphthalene, anthracene, phenantrene

Cyclohexane

Hydrocarbon + salt generalized parameters

H^+ , NH_4^+ , Li^+ , Na^+ , K^+ , Mg^{2+} , Ca^{2+} , Cl^- , OH^- , HCO_3^- , CO_3^{2-} , NO_3^- , SO_4^{2-}

17. Organic solvents and their mixtures with water

Alcohols

Methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, cyclohexanol

Glycols

Mono, di- and triethylene, propylene, polyethylene glycols

Phenols

Phenol, catechol

Ketones

Acetone, methylisobutyl ketone

Aldehydes

Butylaldehyde

Carbonates

Diethylcarbonate, propylene carbonate
 Halogen derivatives
 Chloroform, carbon tetrachloride
 Amines (including mixtures with hydrocarbons)
 Alkylamines:
 Primary: methylamine, ethylamine, n-butylamine, cyclohexylamine, thylenediamine,
 3-methoxypropylamine
 Secondary: dimethylamine, diethylamine
 Tertiary: trimethylamine, triethylamine, tri-n-octylamine
 Mixed amines: methylamine – dimethylamine – trimethylamine
 Alkanolamines
 methyldiethanolamine
 Heterocyclic amines
 N-methylpyrrolidone, morpholine, 2,6-dimethylmorpholine
 Aminoacids
 Methionine
 Nitriles
 Acetonitrile
 Amides
 Dimethylacetamide, dimethylformamide

18. Polyelectrolytes

Polyacrylic acid
 Complexes with Cu, Zn, Ca, Fe(II), Fe(III)

19. Mixed-solvent inorganic/organic system

Methanol – salt systems
 Methanol – H^+ – Na^+ – K^+ – Mg^{2+} – Ca^{2+} – Cl^- – CO_3^{2-} – HCO_3^- – SO_4^{2-} – BO_2^- – $HCOO^-$
 – CH_3COO^- – CO_2 – H_2S
 Glycol – salt systems
 Mono, di- and triethylene glycols – H^+ – Na^+ – K^+ – Mg^{2+} – Ca^{2+} – Ba^{2+} – Cl^- – CO_3^{2-} –
 HCO_3^- – SO_4^{2-} – BO_2^- – CH_3COO^- – CO_2 – H_2S
 Ethanol – salt systems
 Ethanol – Li^+ – Na^+ – Cl^-
 Ethanol – O_2
 Phenol - acetone - SO_2 - HFo - HCl – H_2O
 n-Butylaldehyde – $NaCl$ - H_2O
 $LiPF_6$ – diethylcarbonate – propylene carbonate
 Phenol - acetone - SO_2 - HFo - HCl – H_2O
 n-Butylaldehyde – $NaCl$ - H_2O
 $LiPF_6$ – diethylcarbonate – propylene carbonate

20. Mixed-solvent organic systems

HAc – tri-n-octylamine – toluene – H_2O
 HAc – tri-n-octylamine – methylisobutylketone – H_2O
 Dimethylformamide – HFo – H_2O
 MEG – $EtOH$ – H_2O

21. Ionic liquid systems

Cations: 1-ethyl-3-methyl imidazolium (EMIM), 1-butyl-3-methyl imidazolium (BMIM),
Anions: BF_4^- , PF_6^- , SO_3CF_3^- , $\text{N}(\text{SO}_2\text{CF}_3)_2^-$, $\text{N}(\text{CN})_2^-$
Solvents: Water, methanol, toluene, hexane, dichloromethane

Further developments projected by the end of MSE III (12/31/2009)

Thermophysical framework

Development of a new surface tension model

Development of model parameters

Focus group: Refinery overhead consortium (in collaboration with SwRI)

Modeling hydrometallurgical systems (University of Toronto)

Extension of organic acid chemistry

Improvement of systems containing light components at high pressures

Phase II of oil and gas-related chemistry