What is claimed is:

~~1. A method for predicting a partition coefficient for a solute between a~~ petroleum fraction and water, comprising: selecting a solute class for a solute; determining a solubility constant of water in a petroleum fraction; calculating a solute activity factor based on the solubility constant of water in the petroleum fraction, a solubility constant of the solute in water, a partition coefficient for the solute in octanol and water, and the solute class; and predicting a partition coefficient for the solute in the petroleum fraction and water based on the partition coefficient for the solute in octanol and water, the solute activity factor, and a scaling factor based on the solubility constant of water in the petroleum fraction.

2. A method for predicting a partition coefficient for a solute between a solvent and water, comprising: identifying a plurality of solute classes; fitting parameters for determining a slope in a linear or quasi-linear relationship between a partition coefficient in a solvent and water and a corresponding partition coefficient in octanol and water, the parameters for determining the slope corresponding to coefficients in a polynomial expression based on a solubility constant of water in the solvent, the fitting of parameters being based on a plurality of solvent-water systems; selecting a solute class for a solute; determining a solubility constant of water in a solvent, the solvent being different from solvents in the plurality of solvent-water systems; calculating a solute activity factor based on the solubility constant of water in the solvent, a solubility constant of the solute in water, a partition coefficient for the solute in octanol and water, and the solute class; and predicting a partition coefficient for the solute in the solvent and water based on the partition coefficient for the solute in octanol and water, the solute activity factor, and a scaling factor based on the solubility constant of water in the solvent.

3. A method according to claim 2, wherein the polynomial expression is a quadratic polynomial.

4. A method according to claims 2 or 3, wherein fitting parameters further comprises fitting parameters for determining an intercept value for the linear or quasi-linear relationship, the parameters for determining the intercept value corresponding to coefficients in a polynomial expression based on a solubility constant of water in the ~~solvent, the fitting of parameters being based on a plurality of solvent-water systems.~~

~~5. A method according to any of claims 1 – 4, wherein the solubility constant of~~ water in the petroleum fraction or solvent is determined by measuring a solubility of water in the petroleum fraction or solvent.

6. A method according to any of claims 1 – 5, wherein the scaling factor based on the solubility constant of water in the petroleum fraction corresponds to a slope for a linear or quasi-linear relationship between the partition coefficient for the solute in the petroleum fraction and water and the partition coefficient for the solute in octanol and water.

7. A method according to any of claims 1 – 6, wherein the solute activity factor comprises a scaling factor based on the solute class and a correlation value, the correlation value being defined by

$$C_{activity} = \frac{\ln(\frac{K_{solute}(water)}{K_{water}(solvent)})}{\log P_{solute}(octanol, water)}$$

where $C_{activity}$ is the correlation value, K_{solute}(water) is the solubility constant of the solute in water, K_{water}(solvent) is the solubility constant of water in the petroleum fraction, and P_{solute}(octanol,water) is the partition coefficient of the solute in octanol and water.

8. A method according to any of claims 1 – 7, wherein the partition coefficient for the solute in the petroleum fraction and water is predicted using the relationship

$$P_{solute}(solvent, water) = A * \lambda_{class} * P_{solute}(octanol, water)$$

where P_{solute}(solvent,water) is the partition coefficient of the solute in the petroleum fraction and water, P_{solute}(octanol,water) is the partition coefficient of the solute in octanol and water, A is the scaling factor based on the solubility constant of water in the petroleum fraction, and λ_{class} is $\alpha * C_{activity}$, with the value of α being dependent on the solute class, and wherein the scaling factor A corresponds to

$$A = a * [logK_{water}(solvent)]^2 + b * logK_{water}(solvent) + c$$

where K_{water}(solvent) is the solubility constant of water in the petroleum fraction and a, b, and c are parameters determined based on parameter fitting using a plurality of solvents.

9. A method according to any of claims 1 – 7, wherein the partition coefficient ~~for the solute in the petroleum fraction and water is predicted using the relationship~~

$$P_{solute}(solvent, water) = A * \lambda_{class} * P_{solute}(octanol, water) + B$$

where P_{solute}(solvent,water) is the partition coefficient of the solute in the petroleum fraction and water, P_{solute}(octanol,water) is the partition coefficient of the solute in octanol and water, A is the scaling factor based on the solubility constant of water in the petroleum fraction, B is a factor based on the solubility constant of water in the petroleum fraction, and λ_{class} is α * $C_{activity}$, with the value of α being dependent on the solute class, and wherein the scaling factor B corresponds to

$$B = f * logK_{water}(solvent) + g$$

where K_{water}(solvent) is the solubility constant of water in the petroleum fraction and f and g are parameters determined based on parameter fitting using a plurality of solvents.

10. A method according to any of claims 1 – 9, wherein the petroleum fraction or solvent consists essentially of oil derived from a mineral source.

11. A method according to any of claims 1 – 10, wherein the solute class is selected from a first class for solutes containing nitrogen, a second class for solutes containing sulfur, an acidic functional group, or a hydroxyl functional group, and a class for solutes not assigned to the first class or second class.

12. A method according to claim 11, wherein a solute assigned to the first class for solutes containing nitrogen is not considered for assignment to the second class for solutes containing sulfur or an acidic functional group.

13. A method according to any of claims 1 – 12, wherein the solute is a corrosion inhibitor, a scale inhibitor, or a compound for inhibiting formation of gas hydrates.

What is claimed is:

1. A method for predicting a partition coefficient for a solute between a petroleum fraction and water, comprising:

selecting a solute class for a solute;

obtaining a sample of a petroleum fraction;

determining a solubility constant of water in the petroleum fraction;

calculating a solute activity factor based on the solubility constant of water in the petroleum fraction, a solubility constant of the solute in water, a partition coefficient for the solute in octanol and water, and the solute class; wherein the solubility constant of water in the petroleum fraction is determined by measuring a solubility of water in the petroleum fraction; wherein the solute activity factor comprises a scaling factor based on the solute class and a correlation value, the correlation value being defined by

$$C_{activity} = \frac{\ln\left(\frac{K_{solute}(water)}{K_{water}(solvent)}\right)}{\log P_{solute}(octanol, water)}$$

where $C_{activity}$ is the correlation value, K_{solute}(water) is the solubility constant of the solute in water, K_{water}(solvent) is the solubility constant of water in the petroleum fraction, and P_{solute}(octanol,water) is the partition coefficient of the solute in octanol and water;

predicting a partition coefficient for the solute in the petroleum fraction and water based on the partition coefficient for the solute in octanol and water, the solute activity factor, and a scaling factor based on the solubility constant of water in the petroleum fraction; and

adding the solute to the petroleum fraction based on the predicted partition coefficient.

2. The method of claim 1, wherein the scaling factor based on the solubility constant of water in the petroleum fraction corresponds to a slope for a linear or quasi-linear relationship between the partition coefficient for the solute in the petroleum fraction and water and the partition coefficient for the solute in octanol and water.

3. The method of claim 1, wherein the partition coefficient for the solute in the petroleum fraction and water is predicted using the relationship

$$P_{solute}(solvent, water) = A * \lambda_{class} * P_{solute}(octanol, water)$$

where P_{solute}(solvent,water) is the partition coefficient of the solute in the petroleum fraction and water, P_{solute}(octanol,water) is the partition coefficient of the solute in octanol and water, A is the scaling factor based on the solubility constant of water in the petroleum fraction, and λclass is $\alpha * C_{activity}$, with the value of a being dependent on the solute class.

4. The method of claim 3, wherein the scaling factor A corresponds to A=a*[log

$$A = a * [logK_{water}(solvent)]^2 + b * logK_{water}(solvent) + c$$

where K_{water}(solvent) is the solubility constant of water in the petroleum fraction and a, b, and c are parameters determined based on parameter fitting using a plurality of solvents.

5. The method of claim 1, wherein the partition coefficient for the solute in the petroleum fraction and water is predicted using the relationship

$$P_{solute}(solvent, water) = A * \lambda_{class} * P_{solute}(octanol, water) + B$$

where P_{solute}(solvent,water) is the partition coefficient of the solute in the petroleum fraction and water, P_{solute}(octanol,water) is the partition coefficient of the solute in octanol and water, A is the scaling factor based on the solubility constant of water in the petroleum fraction, B is a factor based on the solubility constant of water in the petroleum fraction, and λclass is $\alpha * C_{activity}$, with the value of a being dependent on the solute class.

6. The method of claim 5, wherein the scaling factor B corresponds to

$$B = f * logK_{water}(solvent) + g$$

where K_{water}(solvent) is the solubility constant of water in the petroleum fraction and f and g are parameters determined based on parameter fitting using a plurality of solvents.

7. The method of claim 1, wherein the petroleum fraction consists essentially of oil derived from a mineral source.

8. The method of claim 1, wherein the solute class is selected from a first class for solutes containing nitrogen, a second class for solutes containing sulfur, or an acidic functional group, or

a hydroxyl functional group, and a third class for solutes not assigned to the first class or second class.

9. The method of claim 8, wherein a solute assigned to the first class for solutes containing nitrogen is not considered for assignment to the second class for solutes containing sulfur or an acidic functional group.

10. The method of claim 1, wherein the solute is a corrosion inhibitor, a scale inhibitor, or a compound for inhibiting formation of gas hydrates.

11. A method for predicting a partition coefficient for a solute between a solvent and water, comprising:

identifying a plurality of solute classes;

fitting parameters for determining a slope in a linear or quasi-linear relationship between a partition coefficient in a solvent and water and a corresponding partition coefficient in octanol and water, the parameters for determining the slope corresponding to coefficients in a polynomial expression based on a solubility constant of water in the solvent, the fitting of parameters being based on a plurality of solvent-water systems;

selecting a solute class for a solute;

determining a solubility constant of water in a solvent, the solvent being different from solvents in the plurality of solvent-water systems;

calculating a solute activity factor based on the solubility constant of water in the solvent, a solubility constant of the solute in water, a partition coefficient for the solute in octanol and water, and the solute class; wherein the solute activity factor comprises a scaling factor based on the solute class and a correlation value, the correlation value being defined by

$$C_{activity} = \frac{\ln\left(\frac{K_{solute}(water)}{K_{water}(solvent)}\right)}{\log P_{solute}(octanol, water)}$$

where $C_{activity}$ is the correlation value, $K_{solute}(water)$ is the solubility constant of the solute in water, $K_{water}(solvent)$ is the solubility constant of water in the solvent, and $P_{solute}(octanol,water)$ is the partition coefficient of the solute in octanol and water; and

predicting a partition coefficient for the solute in the solvent and water based on the partition coefficient for the solute in octanol and water, the solute activity factor, and a scaling factor based on the solubility constant of water in the solvent; and

adding the solute to the solvent based on the predicted partition coefficient.

12. The method of claim 11, wherein the solvent comprises a petroleum fraction.

13. The method of claim 11, wherein the polynomial expression is a quadratic polynomial.

14. The method of claim 11, wherein fitting parameters further comprises fitting parameters for determining an intercept value for the linear or quasi-linear relationship, the parameters for determining the intercept value corresponding to coefficients in a polynomial expression based on a solubility constant of water in the solvent, the fitting of parameters being based on a plurality of solvent-water systems.

15. The method of claim 11, wherein the solute class is selected from a first class for solutes containing nitrogen, a second class for solutes containing sulfur, or an acidic functional group, or a hydroxyl functional group, and a third class for solutes not assigned to the first class or second class.

16. The method of claim 11, wherein partition coefficient for the solute in the solvent and water is predicted using the relationship

$$P_{solute}(solvent, water) = A * \lambda_{class} * P_{solute}(octanol, water) + B$$

where P_{solute}(solvent,water) is the partition coefficient of the solute in the solvent and water, P_{solute}(octanol,water) is the partition coefficient of the solute in octanol and water, A is the scaling factor based on the solubility constant of water in the solvent, B is a factor based on the solubility constant of water in the solvent, and λclass is α*Cactivity, with the value of a being dependent on the solute class.

17. The method of claim 16, wherein the scaling factor A corresponds to

$$A = a * [logK_{water}(solvent)]^2 + b * logK_{water}(solvent) + c$$

where K_{water}(solvent) is the solubility constant of water in the solvent and a, b, and c are parameters determined based on the fitting of parameters.

18. The method of claim 16, wherein the scaling factor B corresponds to

$$B = f * logK_{water}(solvent) + g$$

where K_{water}(solvent) is the solubility constant of water in the solvent and f and g are parameters determined based on the fitting of parameters.