

Project OpSim – Specifications Document

Version 1.0.2

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Preamble

The present document establishes specifications for Open Source Process Simulator (OpSim) project. The effort of development will be segmented in three major areas related to corresponding aspects of the simulator: the user interface, the engine and the data access.

This document is opened for insertions from our development community and will be included in the code repository HTML format, in order that concurrent modifications become feasible.

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1 What is new?

3/17/2006

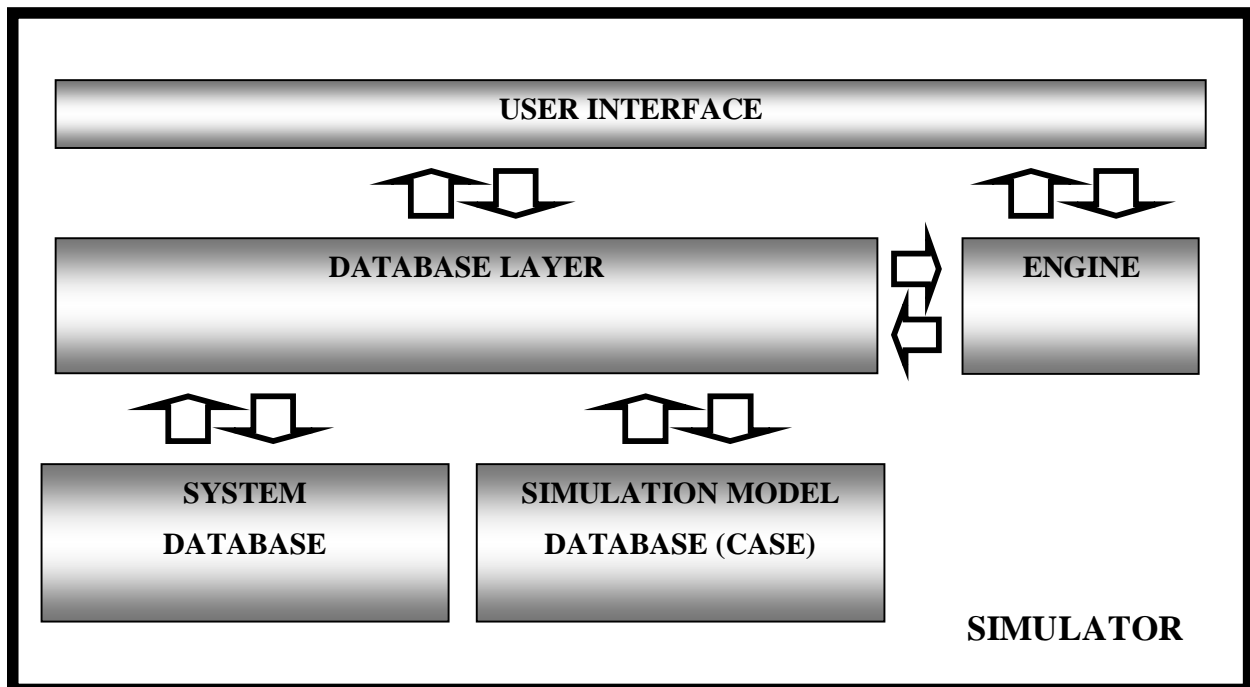
- 1) Updated specs for database files (Samuel)

10/03/2006

- 1) Added schedule proposal (from Hazem).
- 2) Added specs (from Rahul Anantharaman).
- 3) Added structure proposal (from Hazem).

2 Overall Architecture

- 1) The whole simulator structure is divided in three major parts: user interface, engine and data accesses layer. Each one aspect has its own functionality and provides services to each other, through precisely defined boundaries. They exchange information only through these boundaries.
- 2) A diagram illustrating this is shown below:



3 Interface

- 3) The simulator will have an intuitive and friendly graphic user interface (GUI). No development effort is going to be spent in implementing a command line. Interaction with the simulation engine will be provided only through the GUI. An immediate consequence of this approach is that, at the first time, external applications will have no means to use the simulation engine (what would be possible with a command line user interface, using the standard I/O pipes). However there is a remedy to this shortcoming, which does not suffer with the poor performance of communication processes via the use of pipes (see section Engine).
- 4) Fundamental elements of the interface are:
- 5) Component Pallet for unit operations and other components.
- 6) Workspace to build the flow sheet. The Workspace has a drag-drop style, so that elements of the simulation model can be point-clicked and dragged from the Component Pallet
- 7) Report Forms output module.
- 8) Components of a simulation case are defined in the graphical environment through forms. A list of input forms is shown below:

| COMPONENT | DESCRIPTION |
|-----------------------|--|
| Stream | Process stream between two unit ops equipment. |
| Two Phase Separator | |
| Three Phase Separator | |
| Compressor | |
| Valve | |
| Pipe | |
| Heat exchanger | |
| Distillation Column | |
| Pump | |
| Tank | |
| Heater | |
| Cooler | |
| ? | |
| ? | |
| ? | |

4 Engine

- 1) Simulation engine will be steady state. Future version may leverage the models to be transient.
- 2) Simulation engine is closely linked to the user interface, though completely independent of it. This goal may be achieved through an interfacing layer between both.
- 3) With this partition, in a later stage of development, the engine may be packaged in a library (dynamic link library or shared object on Linux) and its interfaces exposed to the system environment. This design permits other applications to directly link and use the simulation engine, completely new user interfaces may be designed even using another programming language.
- 4) The engine comprises basically:
 - 4.1) Solver.
 - 4.2) Mathematical models for each unit operation or simulation component.
 - 4.3) Thermodynamic models.
- 5) Accessing the database is not a functionality of the engine. It does nothing about the database structure. The data needed to solve the simulation are supplied to the engine by other parts of the simulator. After solving the simulation case, the engine supplies the rest of the simulator (interface and database layer) with the partial or final results.

5 Data Access

- 1) The simulator will have input/output (I/O) capabilities to save and reload a simulation case from a file.
- 2) All the data comprising one simulation case is stored in only one file.
- 3) The file I/O operation will be performed through the embedded Relational Database Management System (DBMS): Firebird.
- 4) The technical reasoning to use a DBMS is:
 - 4.1) Low level storage operations are isolated from the simulator.

- 4.2) We do not need to worry about a file format. This is left to the DBMS. If the file format of the DBMS changes, we only need to dump the data and inject in the new version. A custom file format would require exhaustive implementation of converting routines.
 - 4.3) Reliable data storage. DBMS uses sophisticated schemes to access the hard disk in order to protect data.
 - 4.4) Fragmented access to the data file. A custom data file commonly imposes a three stage cycle: reading the file at once, and storing it in the RAM; modifying the data in RAM and writing the whole file at once. DBMS allows read/write small pieces of information in a much more efficient manner.
 - 4.5) Concurrent access to the data in the simulation file. DBMS permits multiple applications accessing the very same simulation case, what is not allowed with a custom formatted file. A simulation case could be built simultaneously by many individuals remotely apart, via the internet, for example, or a local/wide area network (LAN/WAN).
- 5) The technical reasoning to use a Firebird is:
- 5.1) Firebird is an industrial strength DBMS with decades of corporate use.
 - 5.2) Firebird is open source, free of charge, with a very proud active community. The licensing agreement even allows its use with commercial applications, without restrictions (LGPL like).
 - 5.3) Can be easily embedded into the simulator.
 - 5.4) Can be easily scaled up to client/server, allowing simultaneous access of multiple users.
 - 5.5) Available in several operating systems.
 - 5.6) Have a very small footprint and the most advantageous relation [feature set]/[footprint].
 - 5.7) Very fine integration support with Lazarus. Some Delphi components are directly compatible with Lazarus, but regarding the best one (IBObjects), I am not so sure. Anyway, there are native components for a data access in Lazarus.

5.1 Database Structure

- 1) The data utilized by the simulator is stored in two databases:

1.1) System Database: SYSDATA.ODB, used to store intrinsic to the whole system of the simulator, e.g. preferences, environment conjurations, etc. The extension “ODB” stands for “Opsim DataBase”

1.2) Model Database: [model-name].OSC, that store the whole data of the simulation model (case) currently opened at the simulator environment. The extension “OSC” stands for “Opsim Simulation Case”

5.1.1. The System Database

The system database is comprised by the following tables:

- 1) Units of measures used in conversions.
- 2) Sets of units.
- 3) What more???????

1. UNITS OF MEASUREMENT: holds data regarding the units of measurement used in the simulator. This table will be used to build custom sets of units.

| PHISICAL TABLE NAME: UNIT_MEASURE | | | |
|-----------------------------------|--|--------------------------|--------------------|
| FIELD NAME | FIELD DESCRIPTION | FIELD TYPE | FIELD SIZE (BYTES) |
| ID | Internal identification used in referential integrity of the data. | INTEGER (AUTO INCREMENT) | |
| NAME | Name of the unit. | TEXT | 70 |
| SYMBOL | Symbol of the unit in normalized text (e.g. W/m2K or W/m^2.K) | TEXT | 30 |
| CONV_FACTOR_INTERSECT_SI | Intersect conversion factor to the metric system of measurement. | TEXT | 100 |
| CONV_FACTOR_SLOPE_SI | Slope conversion factor to the metric system of | TEXT | 100 |

| | | | |
|--------------------------|--------------|--|--|
| | measurement. | | |
| SOMETHING MORE?????????? | | | |

2. UNIT SETS OF MEASUREMENT: hold unit sets of measurement. A set of units should be used while building the simulation model. Each unit of measurement contained in the set, gets an entry on this table.

| PHISICAL TABLE NAME: UNIT_MEASURE_SET | | | |
|---------------------------------------|--|--------------------------|--------------------|
| FIELD NAME | FIELD DESCRIPTION | FIELD TYPE | FIELD SIZE (BYTES) |
| ID | Internal identification used in referential integrity of the data. | INTEGER (AUTO INCREMENT) | |
| NAME | Name of the unit set (e.g. SI, EuroSI, English System, etc.) | TEXT | 50 |
| UNIT_MEASURE_ID | ID of the unit of measurement. | INTEGER | |
| SOMETHING MORE?????????? | | | |

3. PROPERTIES OF PURE SUBSTANCES: holds data regarding the properties of the pure substances.

| PHISICAL TABLE NAME: PROP_PURE_SUBST | | | |
|--------------------------------------|---|--------------------------|--------------------|
| FIELD NAME | FIELD DESCRIPTION | FIELD TYPE | FIELD SIZE (BYTES) |
| ID | Internal identification used in referential integrity of the data. | INTEGER (AUTO INCREMENT) | |
| CODE | This is a custom code that may be show to the user. It is not used to create relationship between tables of the database. | INTEGER | |

| | | | |
|------------------|--|------|-----|
| NAME | Name of the substance. | TEXT | 70 |
| NAME_IUPAC | IUPAC name o the substance. | TEXT | 100 |
| CHEMICAL_FORMULA | The chemical formula of the substance (e.g. CH ₄) | TEXT | 100 |
| MOLECULAR_WEIGHT | The molecular weight. | REAL | |
| TC | Critical Temperature (K) | REAL | |
| PC | Critical Pressure (Pa) | REAL | |
| VC | Critical Volume (m ³ /kmol) | REAL | |
| API | API gravity | REAL | |
| ACC | Accentic Factor | REAL | |
| NBP | Normal Boiling Point (K) | REAL | |
| VNB | Viscosity at NBP (kgf.hr/m ²) | REAL | |
| HF | Ideal Gas Heat of Formation at Standard temperature (J/kg) | REAL | |
| GF | Ideal Gas Free Energy of Formation at Standard Temperature (J/kg) | REAL | |
| IG_COEFF_1 | Coefficient 1 to calculate Ideal Gas Thermodynamic properties (J/kg) | REAL | |
| IG_COEFF_2 | Coefficient 2 to calculate Ideal Gas Thermodynamic properties (J/kg/K) | REAL | |
| IG_COEFF_3 | Coefficient 3 to calculate Ideal Gas Thermodynamic properties (J/kg/K ²) | REAL | |
| IG_COEFF_4 | Coefficient 4 to calculate Ideal Gas Thermodynamic properties (J/kg/K ³) | REAL | |
| IG_COEFF_5 | Coefficient 5 to calculate | REAL | |

| | | | |
|----------------------------|---|------|--|
| | Ideal Gas Thermodynamic properties (J/kg/K4) | | |
| IG_COEFF_6 | Coefficient 6 to calculate Ideal Gas Thermodynamic properties (J/kg/K5) | REAL | |
| IG_COEFF_7 | Coefficient 7 to calculate Ideal Gas Thermodynamic properties (J/kg/K6) | REAL | |
| SOMETHING MORE????????? | | | |

5.1.2. The Model Database

The model database contains:

- 1) Global options of the simulation model.
- 2) One different table for each type of component added to the model, being it a unit operation, a stream, or whatever.
- 3) Other tables?????
4. PUMPS ON THE SIMULATION MODEL: holds data regarding all the pumps components used in the simulation model. Each pump placed by the user on the PFD diagram, generates a record on this table. Since we may need other tables to keep other others unit operation or components, let establish a prefix now on “PFD_” used to name each table containing unit operation/component of a simulation case.

| PHISICAL TABLE NAME: PFD_PUMP | | | |
|-------------------------------|--|--------------------------|--------------------|
| FIELD NAME | FIELD DESCRIPTION | FIELD TYPE | FIELD SIZE (BYTES) |
| ID | Internal identification used in referential integrity of the data. | INTEGER (AUTO INCREMENT) | |
| CODE | This is a custom code that may be shown to | INTEGER | |

| | | | |
|--------------|---|---------|----|
| | the user. It is not used to create relationship between tables of the database. | | |
| NAME | Descriptive name of the pump. | TEXT | 70 |
| LABEL | Label used to identification on the PFD. | TEXT | 50 |
| HEAD | The head supported by the pump with zero flow rate | REAL | |
| HEAD_UNIT_ID | ID of the unit of measurement used to specify the HEAD field. Needed to do conversions. | INTEGER | |

6 CAPE-OPEN STANDARDS

6.1.1. Standardized Models or Equations (CAPE-OPEN)

This Appendix contains a selection of model equations which may be part of a PPDB. This selection is not meant to be exclusive, every PPDB can add its own equations.

Predictive equations like UNIFAC are exclude on purpose, because they do not need any model parameters.

| short name of method | full name of method | equation | parameters |
|----------------------|---------------------------------|---|---------------|
| Antoine | Antoine vapor pressure equation | $\log(p) = a - b/(T+c)$ | a, b, c |
| Wrede | Wrede vapor pressure equation | $\log(p) = a - b/T$ | a, b |
| Wrede-ln | Wrede vapor pressure equation | $\ln(p) = a - b/T$ | a, b |
| Cragoe | Cragoe vapor pressure equation | $\log(p) = a + b/T + c*T + d*T^2$ | a, b, c, d |
| Riedel | Riedel vapor pressure equation | $\ln(p) = a - b/T + c*T + d*T^2 + e*\ln(T)$ | a, b, c, d, e |

| | | | |
|--------------------|--|---|--|
| Wagner | Wagner vapor pressure equation | $\ln(p/p_{\text{crit}}) = (a*x + b*x_{(3/2)} + c*x^3 + d*x_6)/(T/T_{\text{crit}}); x = 1 - T/T_{\text{crit}}$ | a, b, c, d, criticalPressure, criticalTemperature |
| Wagner2 | 2nd Wagner vapor pressure equation | $\ln(p/p_{\text{crit}}) = (a*x + b*x_{(3/2)} + c*x^3 + d*x_7 + e*x_9)/(T/T_{\text{crit}}); x = 1 - T/T_{\text{crit}}$ | a, b, c, d, e, criticalPressure, criticalTemperature |
| Wagner3 | Wagner vapor pressure equation (Aspen) | $\ln(p/p_{\text{crit}}) = (a*x + b*x_{(3/2)} + c*x^3 + d*x_4)/(T/T_{\text{crit}}); x = 1 - T/T_{\text{crit}}$ | a, b, c, d, criticalPressure, criticalTemperature |
| Chebyshev | Chebyshev vapor pressure equation | $T*\log(p) = c_0/2 + \sum_{(s)}[c_s * E_s(x)]; x = 2*T - (T_{\text{max}}+T_{\text{min}})/(T_{\text{max}}-T_{\text{min}}); E_s(x) = \text{Chebyshev polynomial of order } s$ | c_0, c_1, c_2,, T_min, T_max |
| polynomial | polynomial | $y = a + b*x + c*x^2 + ... + j*x^9$ x = any property | a, b, c, d, e, f, g, h, i, j |
| vapor pressure_1 | vapor pressure equation | $\ln(p) = a + b*T + c/T + d/T^2$ | a, b, c, d |
| mod.Antoine(Hysys) | modified Antoine vapor pressure equation (Hysys[9], page A-36) | $\ln(p) = A + B/(T+C) + D*T + E*\ln(T) + F*T_G$ | A, B, C, D, E, F, G |

| short name of method | full name of method | equation | parameters |
|----------------------------|---|---|---|
| mod.Antoine(Aspen) | modified Antoine vapor pressure equation (Aspen[7], page 3-80) | $\ln(p) = A + B/(T+C) + D*\ln(T) + E*T_F$ | A, B, C, D, E, F |
| Jones-Dole | Jones-Dole equation | $\eta/\eta_0 = 1 + a*\sqrt{c} + b*c$ | a, b, viscosity_0 |
| Yen-Woods | Yen-Woods equation for densities | $d = d_{\text{crit}} * (a + \sum_{(j)}(k_j)*(1 - T/T_{\text{crit}})^{(j/3)})$ | criticalDensity, criticalTemperature, a, k_0, k_1, k_2, ... |
| Antoine viscosity | Antoine equation for the viscosity | $\ln(\eta) = a + b/(T+c)$ | a, b, c |
| Riedel therm.cond. | Riedel equation for thermal conductivities | $\kappa = a * (1 + (20/3)*(1 - T/T_{\text{crit}})^{(2/3)})$ | a, criticalTemperature |
| Sprow/Prausnitz | Surface Tension after Sprow and Prausnitz | $\sigma = a * (1 - T/T_{\text{crit}})^b$ | a, b, criticalTemperature |
| modified polynomial | modified polynomial | property = a + b/T + c/T^2 + d*T + e*T^2 + f*T^3 + ... | a, b, c, d, e, f, ... |
| Yuan/Mok | Yuan - Mok equation for the heat capacity | $c_p = a + b * \exp(-c/T_n)$ | a, b, c, n |
| Redlich-Kister | Redlich-Kister equation for excess properties in binary systems | $\Delta \text{ property} = x_1 * x_2 * \sum_{(i)}(a_i*(x_1 - x_2)^i)$ | a_0, a_1, a_2, a_3, ... |
| thermal conductivity (NEL) | NEL equation for thermal conductivity | $\kappa = a*(1 + b*x_{(1/3)} + c*x_{(2/3)} + d*x); x = 1 - T/T_{\text{crit}}$ | a, b, c, d, criticalTemperature |
| virial equation | virial equation | $Z = 1 + v_{c2}*p + v_{c3}*p^2 + v_{c4}*p^4 + ...$ | vc_2, vc_3, vc_4 |

| | | | |
|------------------------------|--|---|---|
| BWR | BWR-equation of state | $p = R^*T^*d + (b_0^*R^*T - a_0 - c_0/T_2)^*d_2 + (b_0^*R^*T - a_0)^*d_3 + a^*\alpha^*d_6 + (c^*d_3/T_2)^*(1 + \gamma^*d_2)^*\exp(-\gamma^*d_2)$ | $a_0, b_0, c_0, a, b, c, \alpha, \gamma$ |
| BWR-Lee-Starling | Benedict-Webb-Rubin-Lee-Starling equation of state (Aspen ^[7] , page 3-8) | $Z_m = Z_{m0} + \gamma_i^*Z_{m1}; Z_{m0}, Z_{m1} = \text{function}(T, T_{crit}, V_m, V_{crit,m})$ | criticalTemperature_i, criticalVolume_i, gamma_i, epsilon_i_j, eta_i_j |
| Hayden-O'Connel | Hayden-O'Connel equation of state (Aspen ^[7] , page 3-9) | $Z_m = 1 + B^*p/R^*T; B = \sum_{(i)}\sum_{(j)}B_{ij}(T)$ | B_{i_j} |
| Lee-Kesler | Lee-Kesler equation of state (Aspen ^[7] , page 3-18) | $Z = Z_0 + (Z_r - Z_0)^*\omega/\omega_r; Z_0 = f_{ct0}(T/T_{crit}, p/p_{crit}); Z_r = f_{ctr}(T/T_{crit}, p/p_{crit})$ | criticalTemperature, criticalPressure, omega |
| Lee-Kesler-Plöcker | Lee-Kesler-Plöcker equation of state (Aspen ^[7] , page 3-19) | $Z_m = Z_{m0} + (\omega/\omega_r)^*(Z_{m0} - Z_{mr}); Z_{m0} = f_{ct0}(T, T_{crit}, V_m, V_{crit,m}); Z_{mr} = f_{ctr}(T, T_{crit}, V_m, V_{crit,m})$ mixing rules for $V_{crit,m}, T_{crit}$ | criticalTemperature, criticalPressure, vcriticalVolume, omega, Z_{c_i}, K_{i_j} |
| Peng-Robinson-Boston-Mathias | Peng-Robinson-Boston-Mathias equation of state (Aspen ^[7] , page 325) | $p = R^*T/(v_m - b) - a/[v_m^*(v_m + b) + b^*(v_m - b)]$ | criticalTemperature_i, criticalPressure_i, omega_i, k_{1_2} |
| Redlich-Kwong | Redlich-Kwong equation of state (Aspen ^[7] , page 3-27) | $p = R^*T/(v_m - b) - (a/\sqrt{T})/[v_m^*(v_m + b)]$ | criticalTemperature_i, criticalPressure_i |

| short name of method | full name of method | equation | parameters |
|------------------------------------|---|---|---|
| Redlich-Kwong-Aspen | Aspen modification of the Redlich-Kwong equation of state (Aspen ^[7] , page 3-28) | $p = R^*T/(v_m - b) - a/[v_m^*(v_m + b)]$ with mixing rules | criticalTemperature_i, criticalPressure_i, omega_i, $\eta_{i,k_0_a_i_j}, k_{1_a_i_j}, k_{0_D_i_j}, k_{1_D_i_j}$ |
| Redlich-Kwong-Soave-Boston-Mathias | Redlich-Kwong equation of state with Boston-Mathias alpha function (Aspen ^[7] , page 3-29) | $p = R^*T/(v_m - b) - a/[v_m^*(v_m + b)]$ with mixing rules | criticalTemperature_i, criticalPressure_i, omega_i, k_{i_j} |
| Schwartzentruber-Renon | Schwartzentruber-Renon equation of state (Aspen ^[7] , page 3-31) | $p = R^*T/(V_m + c - b) - a/[(v_m + c)^*(V_m + c + b)]$ with mixing rules | criticalTemperature_i, criticalPressure_i, omega_i, $q_{0_i}, q_{1_i}, q_{2_i}, c_{0_i}, c_{1_i}, c_{2_i}, k_{0_a_i_j}, k_{1_a_i_j}, k_{2_a_i_j}, l_{0_i_j}, l_{1_i_j}, l_{2_i_j}, k_{0_D_i_j}, k_{1_D_i_j}, k_{2_D_i_j}$ |
| Peng-Robinson | standard Peng-Robinson equation of state (Aspen ^[7] , page 3-34) | $p = R^*T/(v_m - b) - a/[v_m^*(v_m + b) + b^*(v_m - b)]$ | criticalTemperature_i, criticalPressure_i, omega_i ($i=1..2$), k_{1_2} |
| Redlich-Kwong-Soave | standard Redlich-Kwong-Soave equation of state (Aspen ^[7] , page 335) | $p = R^*T/(v_m - b) - a/[v_m^*(v_m + b)]$ with mixing rules | criticalTemperature_i, criticalPressure_i, omega_i, k_{i_j} |

| | | | |
|-----------------------|--|--|---|
| Bromley-Pitzer | Bromley-Pitzer activity coefficient model (Aspen ^[7] , page 3-54) | | beta_ion, delta_ion, beta_0, beta_1, beta_2, beta_3 |
| Chien-Null | Chien-Null model for calculation activity coefficient of highly non-ideal systems (Aspen ^[7] , page 3-55) | | a_i_j, b_i_j, v_i_j |
| Electrolyte-NRTL | NRTL activity coefficient model for electrolytes(Aspen ^[7] , page 3-58) | | A_B, B_B, C_B, r_i, A_BB, A_BsB, B_BB, B_BsB, alpha_BB, F_BB, F_BsB, G_BB, G_BsB, C_ca_B, C_B_ca, D_ca_B, D_B_ca, E_ca_B, E_B-ca, alpha_ca_B, C_cas_cas, C_cas-cas, c_csa,cssa, C_cssa_csa, D_cas_cas,D_cas_cas, D_csa_cssa, D_cssa_csa, E_cas_cas, E_cas_cas,E_csa_cssa, E_cssa_csa, alpha_cas_cas, alpha_csa_cssa |
| NRTL | NRTL activity coefficient model (DDB ^[8] , page XVI) | | A_i_j, A_j_i, alpha (i,j=1...2) |
| extended NRTL (Aspen) | NRTL activity coefficient model (Aspen ^[7] , page 3-62) | | a_i_j, b_i_j, c_i_j, d_i_j, e_i_j, f_i_j (i,j=1...2) |
| general NRTL | general NRTL activity coefficient model (Hysys ^[9] , page A-22) | | form-of_equation, A_j_j, B_i_j, C_i_j, F_i_j, G_i_j, alpha1_i_j, alpha2_i_j (i,j=1...2) |
| Pitzer activity | Pitzer model for activity | | beta_0, beta_1, beta_2, |

| short name of method | full name of method | equation | parameters |
|----------------------|---|---|---|
| coefficient model | coefficients of aqueous systems (Aspen ^[7] , page 3-63) | | beta_3, C_p, theta_c_cs, theta_a_as, psi_c_cs_a, psi_c_a_as |
| Redlich-Kister | Redlich-Kister model for calculating activity coefficients (Aspen ^[7] , page 3-66) | | a_i_j, b_i_j, c_i_j, d_i_j, e_i_j, f_i_j, g_i_j, h_i_j, m_i_j, n_i_j, v_i |
| Scatchard-Hildebrand | Scatchard-Hildebrand model (Aspen ^[7] , page 3-67) | | critical/Temperature-i, delta_i, V_i_CVT, V_i_l |
| Margules | Margules equation for calculating liquid activity coefficients (DDB ^[8] , page XVI) | $\ln(\gamma_i) = [A_{ij} + 2*(A_{ji}-A_{ij})*x_i](1-x_i)^2$ | A_i_j |
| extended Margules | Margules equation for calculating liquid activity coefficients with temperature-independent parameters (Hysys ^[9] , page A-24) | $\ln(\gamma_i) = (1-x_i)^2 + 2*[A_i + 2*x_i*(B_i-A_i)]$; $A_i = \sum_j [x_j*(a_{ij}+b_{ij}*T)/(1-x_i)]$; $B_i = \sum_j [x_j*(a_{ji}+b_{ji}*T)/(1-x_i)]$ | a_i_j, b_i_j (i,j=1...2) |

| | | | |
|---------------------------|--|--|--|
| three-suffix Margules | extended Margules equation for calculating liquid activity coefficients (Aspen ^[7] , page 3-68) | | $a_{i-j}, b_{i-j}, c_{i-j}, d_{i-j}$ (i,j=1...2) |
| van Laar | van Laar equation for calculating liquid activity coefficients (DDB ^[8] , page XVI) | | A_{i-j} (i,j=1...2) |
| extended van Laar (Aspen) | extended van Laar equation for calculating liquid activity coefficients with temperature-independent parameters (Aspen ^[7] , page 3-75) | | $a_{i-j}, b_{i-j}, c_{i-j}, d_{i-j}$ (i,j=1...2) |
| extended van Laar (Hysys) | extended van Laar equation for calculating liquid activity coefficients with temperature-independent parameters (Hysys ^[9] , page A-28) | | a_{i-j}, b_{i-j} (i,j=1...2) |
| Wilson | Wilson equation for calculating liquid activity coefficients (DDB ^[8] , page XVI) | | A_{i-j} (i,j=1...2) |
| extended Wilson (Aspen) | extended Wilson equation for calculating liquid activity (Aspen ^[7] , page 3-78) | | $a_{i-j}, b_{i-j}, c_{i-j}, d_{i-j}$ (i,j=1...2) |
| extended Wilson (Hysys) | extended Wilson equation for calculating liquid activity coefficients with temperature-independent parameters (Hysys ^[9] , page A-29) | | a_{i-j}, b_{i-j} (i,j=1...2) |
| UNIQUAC | UNIQUAC equation for calculating liquid activity coefficients (DDB ^[8] , page XVII) | | u_{i-j} (i,j=1...2) |
| extended UNIQUAC (Aspen) | extended UNIQUAC equation for calculating liquid activity coefficients with temperature-independent parameters (Aspen ^[7] , page 3-74) | | $a_{i-j}, b_{i-j}, c_{i-j}, d_{i-j}$ (i,j=1...2) |

| short name of method | full name of method | equation | parameters |
|--------------------------|---|--|--------------------------------|
| extended UNIQUAC (Hysys) | extended UNIQUAC equation for calculating liquid activity coefficients with temperature-independent parameters (Hysys ^[9] , page A-26) | | a_{i-j}, b_{i-j} (i,j=1...2) |
| DIPPR107 | DIPPR equation for the ideal heat capacity | $\text{property} = A + B[C/T/\sinh(C/T)]^2 + D[E/T/\cosh(E/T)]^2$ | A, B, C, D, E |
| heat capacity (ASPEN) | Aspen ^[7] -equation for the solid heat capacity (page 3-102) | $C_p = c_1 + c_2*T + c_3*T^2 + c_4/T + c_5/T^2 + c_6/\sqrt{(T)}$ | c1, c2, c3, c4, c5, c6 |
| Barin | Barin equations for thermophysical property data | $G = a + b*T + c*(T*\ln(T)) + d*T^2 + e*T^3 + f*T^4 + g/T + h/T^2$ | a, b, c, d, e, f, g, h |
| Andrade | Andrade equation for calculating the liquid viscosity | $\ln(\eta) = A + B/T + C*\ln(T)$ | A, B, C |

| | | | |
|--------------------------|--|---|--|
| liquid viscosity (DIPPR) | DIPPR equation for the liquid viscosity | $\ln(\eta) = c_1 + c_2/T + c_3 \ln(T) + c_4 T^{c_5}$ | c_1, c_2, c_3, c_4, c_5 |
| viscosity mixing rule | ASPEN _[7] mixing rule for the liquid viscosity (listed under the heading Andrade/DIPPR, page 3-122) | $\ln(\eta) = \sum_i [x_i \ln(\eta_i)] + \sum_{(i,j)} [(a_{ij} + b_{ij}/T) * x_i * x_j + (c_{ij} + d_{ij}/T) * x_i^2 * x_j^2]$ | $a_{i-j}, b_{i-j}, c_{i-j}, d_{i-j}$ |
| DIPPR102 | DIPPR equation for the gas viscosity at 0 atm pressure and the gas thermal conductivity | $\text{property} = A * T_B / (1 + C/T + D/T^2)$ | A, B, C, D |
| Chung-Lee-Starling | Chung-Lee-Starling correlation of the viscosity and thermal conductivity of liquid or gaseous mixtures (Aspen _[7] , page 3-127, 3-138)) | | $\text{criticalTemperature}_i, V_{\text{crit}_i}, \text{dipole_moment}_i, \text{omega}_i, \text{kappa}_i, \text{xi}_{i-j}, \text{zeta}_{i-j}$ |
| surface tension (DIPPR) | DIPPR correlation for surface tension | $\sigma = c_1 * (1 - T_r)^{c_2 + c_3 * T_r + c_4 * T_r^2 + c_5 * T_r^3}; T_r = T/T_{\text{crit}}$ | $c_1, c_2, c_3, c_4, c_5, \text{criticalTemperature}$ |
| Hakim-Steinberg-Stiel | Hakim-Steinberg-Stiel equation for the surface tension (Aspen _[7] , page 3-155) | | χ |
| DIPPR105 | | $\text{property} = A/B^{[1 + (1 - T/C)^D]}$ | A, B, C, D |
| DIPPR101 | | $\text{property} = \exp(A + B/T + C \ln(T) + D * T_E)$ | A, B, C, D, E |
| DIPPR106 | | $\text{property} = A * (1 - T_r)^{(B + C * T_r + D * T_r^2)}; T_r = T/T_{\text{crit}}$ | $A, B, C, D, \text{criticalTemperature}$ |
| DIPPR104 | | $\text{property} = A + B/T + C/T^3 + D/T^8 + E/T^9$ | A, B, C, D, E |

Glossary of the symbols used in the column "equation"

c_p heat capacity d density

d_{crit} critical density p

pressure p_{crit} critical pressure

R gas constant T

temperature T_{crit} critical

temperature v_m volume of a

mixture x_1 mole fraction of

compound 1 Z

compressibility factor Z_m

compressibility factor of a

mixture γ_i activity

coefficient of compound i

κ thermal conductivity

η viscosity η_0 viscosity at

zero concentration σ surface

tension

6.1.2. Standardized Units (CAPE-OPEN)

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|--|---|--------------|---|
| | | no dimension | 1. |
| rad | | | 0.15915475 |
| (BTU.ft ³) ^(1/2) | (J.m ³) ^(1/2) | | 5.4658892 |
| (kJ.m ³) ^(1/2) | (J.m ³) ^(1/2) | | 31.6227766 |
| (J/cm ³) ^(1/2) | (J/c ³) ^(1/2) | | 31.6227766 |
| (BTU/ft ³) ^(1/2) | (J/m ³) ^(1/2) | | 1.9302605E2 |
| (cal/cm ³) ^(1/2) | (J/m ³) ^(1/2) | | 2046.1671 |
| (J/m ³) ^(1/2) | (J/m ³) ^(1/2) | | 1. |
| (kcal/m ³) ^(1/2) | (J/m ³) ^(1/2) | | 64.70548 |
| (g.l) ^(1/2) /min | (kg.m ³) ^(1/2) /s | | 1.6666667E-5 |
| (kg.m ³) ^(1/2) /s | (kg.m ³) ^(1/2) /s | | 1. |
| (lb.ft ³) ^(1/2) /hr | (kg.m ³) ^(1/2) /s | | 3.1481311E-5 |
| (lb.gal) ^(1/2) /min | (kg.m ³) ^(1/2) /s | | 6.9061846E-4 |
| bar.m ⁶ /mol ² | Pa.m ⁶ /mol ² | | 1.E5 |
| bar.m ⁹ .K ² /mol ³ | Pa.m ⁹ .K ² /mol ³ | | 1.E5 |
| bar.m ⁹ /mol ³ | Pa.m ⁹ /mol ³ | | 1.E5 |
| A | A | Ampere | 1. |
| mA | A | | 1.E-3 |
| A/cm ² | A/m ² | | 10000. |
| A/m ² | A/m ² | | 1. |
| mA/cm ² | A/m ² | | 10. |

| | | | |
|-----------------|-----------------|--|-------------|
| mA/m2 | A/m2 | | 0.001 |
| amagat | amagat | | 1. |
| atomic % | atomic fraction | | 0.01 |
| atomic fraction | atomic fraction | | 1. |
| Debye | Coul.m | | 3.33564E-30 |
| Coul | Coul | | 1. |
| Coul.m | Coul.m | | 1. |
| Coul/mol | Coul/mol | | 1. |
| Farad | Farad | | 1. |
| mFarad | Farad | | 0.001 |
| nFarad | Farad | | 1.E-9 |
| pFarad | Farad | | 1.E-12 |
| Farad/m | Farad/m | | 1. |
| oz | g | | 28.349523 |
| H | H | | 1. |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|------------|---------|----------------------|---|
| H/m | H/m | | 1. |
| hr-1 | Hz | | 2.7777778E-4 |
| Hz | Hz | | 1. |
| min-1 | Hz | | 1.6666667E-2 |
| s-1 | Hz | | 1. |
| BTU | J | British thermal unit | 1055.0559 |
| cal | J | | 4.1868 |
| erg | J | | 1.E-7 |
| eV | J | | 1.6021892E-19 |
| GJ | J | | 1.00E9 |
| J | J | | 1. |
| kcal | J | | 4.1868E3 |
| kJ | J | | 1.E3 |
| kp.m | J | | 9.80665 |
| kW.hr | J | | 3.6E6 |
| mJ | J | | 0.001 |
| MMBTU | J | million BTUs | 1.0550559E9 |
| MMkcal | J | million kilocalories | 4.1868E9 |
| erg.mK/cm3 | J.K/m3 | | 0.1 |
| J.K/m3 | J.K/m3 | | 1. |
| kJ/kg.degC | J.kg.K | | 1.0E3 |

| | | | |
|--------------|---------|---|-------------|
| J.s | J.s | | 1. |
| J/Hz | J.s | | 1. |
| J.s/mol | J.s/mol | | 1. |
| BTU/cycle | J/cycle | | 1054.35 |
| cal/cycle | J/cycle | | 4.1868 |
| GJ/cycle | J/cycle | | 1.0E9 |
| J/cycle | J/cycle | | 1. |
| kcal/cycle | J/cycle | | 1000. |
| MMBTU/cycle | J/cycle | | 1.0550559E9 |
| MMkcal/cycle | J/cycle | | 4.1868E9 |
| J/kg.degC | J/g.K | | 1.E-3 |
| J/kg.K | J/g.K | | 1.E-3 |
| kcal/g.degC | J/g.K | | 4.1868E3 |
| BTU/degF | J/K | British thermal unit per degrees Fahrenheit | 1.899101E3 |
| cal/K | J/K | | 4.1868 |
| J/K | J/K | | 1. |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|--------------|---------|--------------------------------------|---|
| kcal/K | J/K | | 4.1868E3 |
| kJ/K | J/K | | 1.E3 |
| kcal/degC.hr | J/K.s | | 1.163 |
| BTU/lb | J/kg | British thermal unit per pound avdp. | 2.32600E3 |
| cal/g | J/kg | | 4.1868E3 |
| cal/g | J/kg | | 4186.8 |
| cal/kg | J/kg | | 4.1868 |
| J/g | J/kg | | 1.E3 |
| J/kg | J/kg | | 1. |
| kcal(th)/kg | J/kg | | 4184. |
| kcal/g | J/kg | | 4186.8E3 |
| kcal/kg | J/kg | | 4186.8 |
| kJ/g | J/kg | | 1.E6 |
| kJ/g | J/kg | | 1.E6 |
| kJ/kg | J/kg | | 1.0E3 |
| kW.hr/ton | J/kg | | 3600. |
| mJ/kg | J/kg | | 0.001 |
| MJ/kg | J/kg | | 1.E6 |

| | | | |
|--------------|--------|------------------------------|-----------|
| MMBTU/lb | J/kg | million BTU per pound (avdp) | 2.32444E9 |
| MMkcal/kg | J/kg | | 4.1868E9 |
| BTU/lb.degF | J/kg.K | | 4.1868E3 |
| BTU/lb.Rnk | J/kg.K | | 4.1868E3 |
| cal(th)/g.K | J/kg.K | | 4148. |
| cal/g.degC | J/kg.K | | 4.1868E3 |
| cal/g.K | J/kg.K | | 4186.8 |
| cal/kg.degC | J/kg.K | | 4.1868 |
| cal/kg.K | J/kg.K | | 4.1868 |
| J/g.degC | J/kg.K | | 1.E3 |
| J/g.K | J/kg.K | | 1.E3 |
| J/kg.K | J/kg.K | | 1. |
| kcal/g.K | J/kg.K | | 4186.8E3 |
| kcal/kg.degC | J/kg.K | | 4186.8 |
| kcal/kg.K | J/kg.K | | 4.1868E3 |
| kcal/kg.K | J/kg.K | | 4186.8 |
| kJ/g.degC | J/kg.K | | 1.E6 |
| kJ/g.K | J/kg.K | | 1.E6 |
| kJ/kg.K | J/kg.K | | 1000. |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|-------------|---------|---------|---|
| BTU/lb.Rnk2 | J/kg.K2 | | 7536.2403 |
| J/kg.K2 | J/kg.K2 | | 1. |
| kcal/kg.K2 | J/kg.K2 | | 4186.8 |
| kJ/g.K2 | J/kg.K2 | | 1.E6 |
| kJ/kg.K2 | J/kg.K2 | | 1000. |
| BTU/lb.Rnk3 | J/kg.K3 | | 13565.2326 |
| kcal/kg.K3 | J/kg.K3 | | 4186.8 |
| kJ/g.K3 | J/kg.K3 | | 1.E6 |
| kJ/kg.K3 | J/kg.K3 | | 1000. |
| BTU/lb.Rnk4 | J/kg.K4 | | 24417.4187 |
| kcal/kg.K4 | J/kg.K4 | | 4186.8 |
| kJ/g.K4 | J/kg.K4 | | 1.E6 |
| kJ/kg.K4 | J/kg.K4 | | 1000. |
| BTU/lb.Rnk5 | J/kg.K5 | | 43951.3537 |
| kcal/kg.K5 | J/kg.K5 | | 4186.8 |
| kJ/g.K5 | J/kg.K5 | | 1.E6 |
| kJ/kg.K5 | J/kg.K5 | | 1000. |

| | | | |
|-------------------|------------|--|--------------|
| J/g.bar | J/kg.Pa | | 0.01 |
| J/kg.Pa | J/kg.Pa | | 1. |
| J/g.bar.K | J/kg.Pa.K | | 0.01 |
| J/kg.Pa.K | J/kg.Pa.K | | 1. |
| J/g.bar2.K | J/kg.Pa2.K | | 1.E-7 |
| J/kg.Pa2.K | J/kg.Pa2.K | | 1. |
| BTU/ft.hr | J/m.s | | 0.96150757 |
| cal/m.s | J/m.s | | 4.1868 |
| J/m.s | J/m.s | | 1. |
| MMBTU/hr.ft | J/m.s | | 0.96150757E6 |
| BTU.ft/ft2.hr.Rnk | J/m.s.K | | 0.09495505 |
| BTU/ft.hr.degF | J/m.s.K | | 1.730734744 |
| cal.cm/s.cm2.K | J/m.s.K | | 418.68 |
| kcal/m.hr.degC | J/m.s.K | | 1.163 |
| MMBTU/hr.ft2.Rnk | J/m.s.K | | 5.6782633E6 |
| cal/cm2 | J/m2 | | 4.1868E4 |
| erg/cm2 | J/m2 | | 1.E-3 |
| J/cm2 | J/m2 | | 1.E4 |
| J/m2 | J/m2 | | 1. |
| kcal/m2 | J/m2 | | 4.1868E3 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|-----------------|----------|---------|---|
| kJ/m2 | J/m2 | | 1.E3 |
| BTU/ft2.hr.Rnk | J/m2.K | | 5.6782636 |
| cal/cm2.K | J/m2.K | | 4.1868E4 |
| cal/m2.K | J/m2.K | | 4.1868 |
| J/cm2.K | J/m2.K | | 1.E4 |
| J/m2.K | J/m2.K | | 1. |
| kcal/m2.K | J/m2.K | | 4.1868E3 |
| kJ/m2.K | J/m2.K | | 1.E3 |
| BTU/ft2.hr | J/m2.s | | 3.1545909 |
| BTU/ft2.hr.degF | J/m2.s.K | | 5.6782636 |
| J/m2.s.K | J/m2.s.K | | 1.0 |
| BTU/ft3 | J/m3 | | 29.875856 |
| cal/cm3 | J/m3 | | 4.1868E6 |
| J/m3 | J/m3 | | 1. |
| kcal/m3 | J/m3 | | 4.1868E3 |
| kJ/cm3 | J/m3 | | 1000. |

| | | | |
|--------------|--------|---------------------------------------|-----------|
| kJ/m3 | J/m3 | | 1.0E3 |
| BTU/ft3.Rnk | J/m3.K | | 53.776541 |
| cal/cm3.K | J/m3.K | | 4.1868E6 |
| J/cm3.K | J/m3.K | | 1000000. |
| J/m3.K | J/m3.K | | 1. |
| kcal/m3.K | J/m3.K | | 4.1868E3 |
| kJ/m3.K | J/m3.K | | 1000. |
| BTU/lbmol | J/mol | British thermal units per pound-moles | 2.326E3 |
| BTU/mol | J/mol | | 1055.056 |
| cal(th)/mol | J/mol | | 4.184 |
| cal/kmol | J/mol | | 4.1868E3 |
| cal/mol | J/mol | | 4.1868 |
| GJ/kmol | J/mol | | 1.0E12 |
| J/kmol | J/mol | | 0.001 |
| J/mol | J/mol | | 1. |
| kcal(th)/mol | J/mol | | 4.184E3 |
| kcal/kmol | J/mol | | 4.1868 |
| kcal/mol | J/mol | | 4.1868E3 |
| kJ/kmol | J/mol | | 1.0 |
| kJ/mol | J/mol | | 1000. |
| MJ/kmol | J/mol | | 1000. |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|----------------|---------|---------|---|
| MMBTU/lbmol | J/mol | | 2.32444E6 |
| MMkcal/mol | J/mol | | 4.1868E9 |
| BTU/lbmol.degF | J/mol.K | | 4.1868 |
| BTU/lbmol.Rnk | J/mol.K | | 4.1868 |
| BTU/mol.F | J/mol.K | | 1.8991006E3 |
| BTU/mol.Rnk | J/mol.K | | 1.8991006E3 |
| cal(th)/mol.K | J/mol.K | | 4.184 |
| cal/kmol.degC | J/mol.K | | 4.1868E3 |
| cal/kmol.K | J/mol.K | | 4.1868E3 |
| cal/mol.degC | J/mol.K | | 4.1868 |
| cal/mol.K | J/mol.K | | 4.1868 |
| cal/mol.K | J/mol.K | | 4.1868 |
| J/kmol.degC | J/mol.K | | 0.001 |
| J/kmol.K | J/mol.K | | 0.001 |

| | | | |
|----------------|----------|--|----------|
| J/mol.degC | J/mol.K | | 1. |
| J/mol.K | J/mol.K | | 1 |
| kcal/kmol.degC | J/mol.K | | 4.1868 |
| kcal/kmol.K | J/mol.K | | 4.1868 |
| kcal/mol.degC | J/mol.K | | 4.1868E3 |
| kcal/mol.K | J/mol.K | | 4.1868E3 |
| kJ/kmol.degC | J/mol.K | | 1. |
| kJ/kmol.K | J/mol.K | | 1. |
| kJ/mol.degC | J/mol.K | | 1000. |
| kJ/mol.K | J/mol.K | | 1.E3 |
| BTU/lbmol.Rnk2 | J/mol.K2 | | 7.53624 |
| cal(th)/mol.K2 | J/mol.K2 | | 4.184 |
| cal/mol.K2 | J/mol.K2 | | 4.1868 |
| J/mol.K2 | J/mol.K2 | | 1. |
| kcal/kmol.K2 | J/mol.K2 | | 4.1868 |
| kJ/kmol.K2 | J/mol.K2 | | 1. |
| kJ/mol.K2 | J/mol.K2 | | 1000. |
| cal(th)/mol.K3 | J/mol.K3 | | 4.184 |
| cal/mol.K3 | J/mol.K3 | | 4.1868 |
| J/mol.K3 | J/mol.K3 | | 1. |
| kJ/mol.K3 | J/mol.K3 | | 1000. |
| cal(th)/mol.K4 | J/mol.K4 | | 4.184 |
| J/mol.K4 | J/mol.K4 | | 1. |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|----------------|------------|---------|---|
| cal/mol.atm | J/mol.Pa | | 4.13205E-5 |
| J/mol.Pa | J/mol.Pa | | 1. |
| cal/mol.Torr.K | J/mol.Pa.K | | 0.0314035751 |
| J/mol.Pa.K | J/mol.Pa.K | | 1. |
| BTU/hr | J/s | | 0.29307107 |
| cal/hr | J/s | | 1.163E-3 |
| cal/s | J/s | | 4.1868 |
| GJ/hr | J/s | | 2.7777778E5 |
| J/s | J/s | | 1. |
| kcal/hr | J/s | | 1.1629833 |
| kJ/hr | J/s | | 0.277777778 |
| kJ/min | J/s | | 16.666667 |
| kJ/s | J/s | | 1.0E3 |

| | | | |
|-----------------|----------|--------------------|---------------|
| MJ/hr | J/s | | 277.77778 |
| MMBTU/day | J/s | | 1.221129458E4 |
| MMBTU/hr | J/s | | 0.29307107E6 |
| MMkcal/day | J/s | | 4.84576375E4 |
| MMkcal/hr | J/s | | 1.1629833E6 |
| BTU/hr.degF | J/s.K | | 0.52753056 |
| BTU/hr.Rnk | J/s.K | | .527527926 |
| cal/s.K | J/s.K | | 4.1868 |
| J/s.K | J/s.K | | 1. |
| kcal/hr.K | J/s.K | | 1.1629833 |
| kcal/s.K | J/s.K | | 4186.8 |
| kJ/hr.degC | J/s.K | | 0.27777778 |
| kJ/s.degC | J/s.K | | 1.0E3 |
| kJ/s.K | J/s.K | | 1.0E3 |
| kcal/hr.m2 | J/s.m2 | | 1.1629833 |
| kJ/hr.m2 | J/s.m2 | | 0.277777778 |
| kJ/s.m2 | J/s.m2 | | 1000. |
| kJ/s.m2.K | J/s.m2 | | 1.0E3 |
| kcal/hr.m2.degC | J/s.m2.K | | 1.1629833 |
| kcal/hr.m2.K | J/s.m2.K | | 1.1629833 |
| kcal/s.m2.K | J/s.m2.K | | 4186.8 |
| kJ/hr.m2.degC | J/s.m2.K | | 0.277777778 |
| kJ/s.m2.degC | J/s.m2.K | | 1000. |
| degC | K | degrees centigrade | 1. (+273.15) |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|-----------|---------|---------|---|
| degF | K | | 0.55555556 (+255.37222) |
| K | K | | 1. |
| kK | K | | 1000. |
| mK | K | | 0.001 |
| Reamur | K | | 1.25 (+273.15) |
| Rnk | K | | 0.55555556 |
| degF/psia | K/Pa | | 8.05764E-5 |
| K/atm | K/Pa | | 9.86923E-6 |
| K/bar | K/Pa | | 1.E-5 |
| K/MPa | K/Pa | | 1.E-6 |
| K/Pa | K/Pa | | 1. |
| degC-1 | K-1 | | 1. |

| | | | |
|------------------|----------|--------------------|--------------|
| degF-1 | K-1 | | 1.8 |
| K-1 | K-1 | | 1. |
| Rnk-1 | K-1 | | 1.8 |
| K2 | K2 | | 1. |
| degF2/lbmol2 | K2/mol2 | | 1.500111E-6 |
| degF2/lbmol3 | K2/mol3 | | 3.3071795E-9 |
| K2/Pa | K2/Pa | | 1. |
| K2/Torr | K2/Pa | | 7.500615E-3 |
| K3 | K3 | | 1. |
| g | kg | | 0.001 |
| kg | kg | | 1. |
| lb | kg | pound avdp. | 0.45359237 |
| Mlb | kg | 1000 pounds (avdp) | 453.59237 |
| ton | kg | | 1000. |
| ton(long) | kg | | 1016.0469 |
| ton(short) | kg | | 907.18474 |
| kg.m2 | kg.m2 | | 1. |
| lb.in2 | kg.m2 | | 2.9263961E-4 |
| g/cycle | kg/cycle | | 0.001 |
| kg/cycle | kg/cycle | | 1. |
| lb/cycle | kg/cycle | | 0.45359237 |
| Mlb/cycle | kg/cycle | | 453.59237 |
| ton(short)/cycle | kg/cycle | | 907.18474 |
| ton/cycle | kg/cycle | | 1000. |
| kg/J | kg/J | | 1. |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|----------------|---------------|--------------------------|---|
| g/100g solvent | kg/kg solvent | | 0.01 |
| g/kg solvent | kg/kg solvent | | 0.001 |
| kg/kg solvent | kg/kg solvent | kg solute per kg solvent | 1. |
| mg/kg solvent | kg/kg solvent | | 1.E-6 |
| kg/m | kg/m | | 1. |
| lb/ft | kg/m | | 1.4881639 |
| kg/m.hr | kg/m.s | | 2.7777778E-4 |
| slug/hr.ft | kg/m.s | | 0.013268619 |
| kg/m.hr2 | kg/m.s2 | | 7.7160494E-8 |
| kg/m.s2 | kg/m.s2 | | 1. |
| lb/in.s2 | kg/m.s2 | | 17.857967 |

| | | | |
|---------------|------------|--|--------------|
| lb/m.s2 | kg/m.s2 | | 0.45359237 |
| g.cm2 | kg/m2 | | 10. |
| kg/cm2 | kg/m2 | | 1.E-4 |
| kg/m2 | kg/m2 | | 1. |
| lb.ft2 | kg/m2 | | 0.04214 |
| poundals/ft2 | kg/m2 | | 0.15175047 |
| kg/m2.atm.hr | kg/m2.Pa.s | | 2.7414535E-9 |
| lb/ft2.atm.hr | kg/m2.Pa.s | | 1.3384948E-8 |
| g/cm2.s | kg/m2.s | | 10. |
| kg/m2.hr | kg/m2.s | | 2.7777778E-4 |
| kg/m2.s | kg/m2.s | | 1. |
| lb/ft2.hr | kg/m2.s | | 1.3562298E-3 |
| lb/ft2.s | kg/m2.s | | 4.8824276 |
| g/cm2.s.atm | kg/m2.s.Pa | | 9.8692326E-5 |
| g/cm2.s.Pa | kg/m2.s.Pa | | 10. |
| kg/m2.s.Pa | kg/m2.s.Pa | | 1. |
| g/100ml | kg/m3 | | 10. |
| g/cm3 | kg/m3 | | 1000. |
| g/dm3 | kg/m3 | | 1. |
| g/l | kg/m3 | | 1. |
| g/m3 | kg/m3 | | 1.E-3 |
| g/ml | kg/m3 | | 1.E3 |
| kg/cm3 | kg/m3 | | 1.E6 |
| kg/dm3 | kg/m3 | | 1.E3 |
| kg/l | kg/m3 | | 1.E3 |
| kg/m3 | kg/m3 | | 1. |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|-------------------|-------------------|--------------------------|---|
| lb/ft3 | kg/m3 | | 16.018463 |
| lb/gal | kg/m3 | | 119.82643 |
| lb/in3 | kg/m3 | | 27.6799E3 |
| mg/cm3 | kg/m3 | | 1. |
| mg/l | kg/m3 | | 1.E-3 |
| mg/m3 | kg/m3 | | 1.E-6 |
| g/100cm3 solvent | kg/m3 solvent | | 10. |
| g/l solvent | kg/m3 solvent | | 1. |
| kg/m3 solvent | kg/m3 solvent | kg solute per m3 solvent | 1. |
| kg/m3(0 C, 1 atm) | kg/m3(0 C, 1 atm) | kg per norm cubic m | 1. |

| | | | |
|---------------------------------|-----------------------|--|--------------|
| g/cm ³ .K | kg/m ³ .K | | 1.E3 |
| kg/m ³ .K | kg/m ³ .K | | 1. |
| g/mol | kg/mol | | 0.001 |
| kg/mol | kg/mol | | 1. |
| lb/lb(force).hr.ft ² | kg/N.s.m ² | | 3.0489259E-4 |
| g/atm.hr | kg/Pa.s | | 2.7414535E-6 |
| g/bar.hr | kg/Pa.s | | 2.7777778E-6 |
| g/kPa.hr | kg/Pa.s | | 2.7777778E-4 |
| g/kPa.min | kg/Pa.s | | 1.6666667E-8 |
| g/kPa.s | kg/Pa.s | | 1.E-6 |
| g/mmHg.hr | kg/Pa.s | | 2.0835042E-3 |
| kg/atm.hr | kg/Pa.s | | 2.7414535E-9 |
| kg/atm.s | kg/Pa.s | | 9.8692327E-6 |
| kg/bar.hr | kg/Pa.s | | 2.7777778E-9 |
| kg/bar.s | kg/Pa.s | | 1.E-5 |
| kg/cmH ₂ O.hr | kg/Pa.s | | 2.8326244E-6 |
| kg/kPa.hr | kg/Pa.s | | 2.7777778E-7 |
| kg/kPa.min | kg/Pa.s | | 1.6666667E-5 |
| kg/kPa.s | kg/Pa.s | | 1.E-3 |
| kg/mmH ₂ O.hr | kg/Pa.s | | 2.8326244E-7 |
| kg/mmHg.hr | kg/Pa.s | | 2.0835042E-6 |
| kg/Pa.hr | kg/Pa.s | | 2.7777778E-4 |
| lb/atm.hr | kg/Pa.s | | 1.2435024E-9 |
| lb/atm.s | kg/Pa.s | | 4.4766086E-6 |
| lb/inH ₂ O.hr | kg/Pa.s | | 5.0585892E-7 |
| lb/inHg(32F).hr | kg/Pa.s | | 3.7207138E-8 |
| lb/psi.hr | kg/Pa.s | | 1.827444E-8 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|------------|---------|---------|---|
| lb/psi.min | kg/Pa.s | | 1.0964664E-6 |
| lb/psi.s | kg/Pa.s | | 6.5787985E-5 |
| g/s | kg/s | | 1.E-3 |
| kg/day | kg/s | | 1.157407417E-5 |
| kg/hr | kg/s | | 0.2777778E-3 |
| kg/min | kg/s | | 0.016666667 |
| kg/s | kg/s | | 1. |
| lb/day | kg/s | | 5.249911667E-6 |
| lb/hr | kg/s | | 0.12599788E-3 |

| | | | |
|--------------|--------------|---------------------------------|--------------|
| lb/s | kg/s | | 453.59237E-3 |
| Mlb/hr | kg/s | 1000 pounds (avdp) per hour | 0.12599788 |
| ton/day | kg/s | | 0.0115741 |
| ton/hr | kg/s | | 0.27777778 |
| ton/year | kg/s | | 3.1709792E-5 |
| kg/kW.hr | kg/W.hr | | 2.777778E-7 |
| lb/hp.hr | kg/W.s | | 1.689659E-7 |
| kg-1.m-1.s-1 | kg-1.m-1.s-1 | | 1. |
| kJ/cycle | kJ/cycle | | 1000. |
| l/Val | l/Val | | 1. |
| Ang | m | Angstrøm | 1.E-10 |
| cm | m | | 0.01 |
| dm | m | | 0.1 |
| ft | m | | 0.3048 |
| in | m | | 0.0254 |
| km | m | | 1000. |
| m | m | | 1. |
| micron | m | | 1.E-6 |
| mile | m | | 1609.344 |
| mm | m | | 1.E-3 |
| nm | m | | 1.E-9 |
| um | m | mikro-meter | 1.E-6 |
| yd | m | | 0.9144 |
| m/K | m/K | | 1. |
| ft/lb | m/kg | | 6.719690E-1 |
| m/kg | m/kg | | 1. |
| bbl/ft2.hr | m/s | barrel per square foot and hour | 4.7535474E-4 |
| cm/hr | m/s | | 2.777778E-6 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|-----------|---------|---------|---|
| cm/s | m/s | | 0.01 |
| cm2/cm.s | m/s | | 0.01 |
| ft/hr | m/s | | 8.46666667E-5 |
| ft/min | m/s | | 5.08E-3 |
| ft/s | m/s | | 0.3048 |
| ft2/ft.hr | m/s | | 8.4666667E-5 |
| ft2/ft.s | m/s | | 0.3048 |
| ft3/ft2.s | m/s | | 0.3048 |

| | | | |
|--------------------------------------|-----------------------------------|--|---------------|
| ft ³ /ft ² .hr | m/s | | 8.46666667E-5 |
| gal/ft ² .min | m/s | | 6.79097E-4 |
| km/hr | m/s | | 0.27777778 |
| km/s | m/s | | 1000. |
| l/m ² .hr | m/s | | 2.7778E-7 |
| l/m ² .s | m/s | | 1.E-3 |
| m/hr | m/s | | 2.77777778E-4 |
| m/min | m/s | | 0.0166666667 |
| m/s | m/s | | 1. |
| m/s | m/s | | 1. |
| m ² /m.hr | m/s | | 2.777778E-4 |
| m ² /m.s | m/s | | 1. |
| m ³ /m ² .s | m/s | | 1. |
| m ³ /m ² .min | m/s | | 1.6666667E-2 |
| mile/hr | m/s | | 0.44704 |
| l/hr.rpm | m/s.rpm | | 2.777778E-7 |
| m ³ /min.rpm | m/s.rpm | | 1.6666667E-2 |
| cm-1 | m-1 | | 100. |
| cm ² /cm ³ | m-1 | | 100. |
| ft-1 | m-1 | | 3.280840 |
| ft ² /ft ³ | m-1 | | 3.2808 |
| in-1 | m-1 | | 39.370079 |
| in ² /in ³ | m-1 | | 0.39370079 |
| m-1 | m-1 | | 1. |
| m ² /m ³ | m-1 | | 1. |
| mm-1 | m-1 | | 1000.0 |
| mm ² /mm ³ | m-1 | | 1000. |
| m-1.s-2 | m-1.s-2 | | 1. |
| cm ¹² /mol ⁴ | m ¹² /mol ⁴ | | 1.E-24 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|------------------------------------|-----------------------------------|---------|---|
| l ⁴ /mol ⁴ | m ¹² /mol ⁴ | | 1.E-12 |
| m ¹² /mol ⁴ | m ¹² /mol ⁴ | | 1. |
| cm ¹⁵ /mol ⁵ | m ¹⁵ /mol ⁵ | | 1.E-30 |
| m ¹⁵ /mol ⁵ | m ¹⁵ /mol ⁵ | | 1. |
| ft-2 | m-2 | | 10.76364864 |
| cm ² | m ² | | 1.E-4 |
| dm ² | m ² | | 0.01 |

| | | | |
|---------------|------------|------------------------|--------------|
| ft2 | m2 | | 0.09290304 |
| in2 | m2 | | 0.00064516 |
| m2 | m2 | | 1. |
| mm2 | m2 | | 1.E-6 |
| nm2 | m2 | | 1.E-18 |
| m2.K/kW | m2.K/W | | 1.0E-3 |
| m2.K/W | m2.K/W | | 1. |
| m2/g | m2/kg | | 0.001 |
| m2/kg | m2/kg | | 1. |
| ft2/lb(force) | m2/N | | 2.0885434E-2 |
| m2/Ohm | m2/Ohm | | 1. |
| cm2/Ohm.mol | m2/Ohm.mol | | 1.E-4 |
| m2/Ohm.mol | m2/Ohm.mol | | 1. |
| Sie.cm2/mol | m2/Ohm.mol | | 0.01 |
| cm2/Ohm.val | m2/Ohm.val | | 1.E-4 |
| m2/Ohm.val | m2/Ohm.val | | 1. |
| bbl/ft.hr | m2/s | barrel/(foot and hour) | 9.1134442E-4 |
| cm2/s | m2/s | | 1.E-4 |
| cSt | m2/s | centistokes | 1.E-6 |
| ft2/hr | m2/s | | 2.58064E-5 |
| ft2/min | m2/s | | 1.548385E-3 |
| ft3/ft.hr | m2/s | | 2.58064E-5 |
| l/hr.m | m2/s | | 2.7777778E-7 |
| m2/day | m2/s | | 1.1574074E-5 |
| m2/hr | m2/s | | 2.7777778E-4 |
| m2/s | m2/s | | 1. |
| m2/year | m2/s | | 3.1688087E-8 |
| m3/m.min | m2/s | | 1.6666667E-2 |
| m3/m.s | m2/s | | 1. |
| mm2/s | m2/s | | 1.E-6 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|--------------------|-------------------|---------|---|
| mSt | m2/s | | 1.E-7 |
| St | m2/s | | 1.E-4 |
| cm2/s.mol fraction | m2/s.mol fraction | | 1. |
| m2/s.mol fraction | m2/s.mol fraction | | 1. |
| m2/s2 | m2/s2 | | 1. |
| cm2/V.s | m2/V.s | | 1.E-4 |

| | | | |
|---------------|----------|------------------------------|----------------|
| m2/V.s | m2/V.s | | 1. |
| bbl | m3 | barrel | 0.15898729 |
| cm3 | m3 | | 1.0E-6 |
| dm3 | m3 | | 1.E-3 |
| ft3 | m3 | | 2.8316847E-2 |
| gal | m3 | | 3.7854118E-3 |
| in3 | m3 | | 1.6387064E-5 |
| l | m3 | liters | 1.E-3 |
| m3 | m3 | | 1. |
| ml | m3 | | 1.E-6 |
| cm3.K/mol | m3.K/mol | | 1.E-6 |
| ft3.Rnk/lbmol | m3.K/mol | | 3.468220043E-5 |
| m3.K/kmol | m3.K/mol | | 1.E-3 |
| bbl/cyle | m3/cycle | barrel/cycle | 0.15898729 |
| ft3/cycle | m3/cycle | | 2.8316847E-2 |
| gal/cycle | m3/cycle | | 3.7854118E-3 |
| kbbl/cycle | m3/cycle | 1000 barrels per cycle | 0.15898729 |
| l/cycle | m3/cycle | | 0.001 |
| m3/cycle | m3/cycle | | 1. |
| MMft3/cycle | m3/cycle | million cubic feet per cycle | 2.8316847E4 |
| kbbl/day | m3/day | | 1.840131E-6 |
| cm3/kg | M3/g | | 1.E-3 |
| m3/K | m3/K | | 1. |
| cm3/100g | m3/kg | | 1.E-5 |
| cm3/g | m3/kg | | 1.E-3 |
| dm3/g | m3/kg | | 1. |
| dm3/kg | m3/kg | | 1.E-3 |
| ft3/lb | m3/kg | | 0.062427962 |
| l/g | m3/kg | | 1. |
| l/kg | m3/kg | | 1.E-3 |
| m3/kg | m3/kg | | 1. |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|---------------|---------------|---------|---|
| ml/g | m3/kg | | 1.E-3 |
| cm3/g solvent | m3/kg solvent | | 1.E-3 |
| m3/kg solvent | m3/kg solvent | | 1. |
| m3/kg.s | m3/kg.s | | 1. |
| m3/kg.s2 | m3/kg.s2 | | 1. |

| | | | |
|---------------------|---------------------|--|-----------------|
| cm3/cm3 solvent | m3/m3 solvent | | 1. |
| cm3/l solvent | m3/m3 solvent | | 1.E-3 |
| l/l solvent | m3/m3 solvent | | 1. |
| m3/m3 solvent | m3/m3 solvent | | 1. |
| ml/ml solvent | m3/m3 solvent | | 1. |
| cm3/cm3(sat.solut.) | m3/m3(sat.solution) | | 1. |
| cm3/l.atm | m3/m3.Pa | | 0.0098692327E-6 |
| m3/m3.Pa | m3/m3.Pa | | 1. |
| dm3/mol | m3/mol | | 1.E-3 |
| ft3/lbmol | m3/mol | | 6.242796029E-5 |
| l/mol | m3/mol | | 1.E-3 |
| m3/kmol | m3/mol | | 0.001 |
| m3/mol | m3/mol | | 1. |
| ml/mol | m3/mol | | 1.E-6 |
| cm3/mol2 | m3/mol2 | | 1.E-6 |
| cm3/bar.g | m3/Pa.kg | | 1.E-8 |
| m3/Pa.kg | m3/Pa.kg | | 1. |
| bbl/psi.hr | m3/Pa.s | barrel/(pounds per square inch and hour) | 6.4053188E-9 |
| ft3/psia.min | m3/Pa.s | | 6.8450163E-8 |
| ft3/psia.s | m3/Pa.s | | 4.107010E-6 |
| l/atm.hr | m3/Pa.s | | 2.7414535E-12 |
| l/kPa.hr | m3/Pa.s | | 2.7777778E-10 |
| l/mmHg.hr | m3/Pa.s | | 2.0835042E-9 |
| m3/kPa.hr | m3/Pa.s | | 2.7777778E-7 |
| m3/kPa.min | m3/Pa.s | | 1.6666667E-5 |
| m3/kPa.s | m3/Pa.s | | 1.E-3 |
| ml/atm.hr | m3/Pa.s | | 2.7414535E-15 |
| ml/kPa.hr | m3/Pa.s | | 2.7777778E-13 |
| bbl/day | m3/s | barrel/day | 1.8401307E-6 |
| bbl/hr | m3/s | barrel/hour | 0.04415E-3 |
| ft3/day | m3/s | | 3.2774128E-7 |
| ft3/hr | m3/s | | 7.8657907E-6 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|---------|---------|---------|---|
| ft3/min | m3/s | | 4.7194744E-4 |
| ft3/s | m3/s | | 0.028316846 |
| gal/hr | m3/s | | 1.0515033E-6 |

| | | | |
|-------------|----------|-----------------------------|----------------|
| gal/min | m3/s | | 6.3090196E-5 |
| l/day | m3/s | | 1.157407E-8 |
| l/hr | m3/s | | 2.7777778E-7 |
| l/min | m3/s | | 1.6666667E-5 |
| l/s | m3/s | | 0.001 |
| l/year | m3/s | | 3.1688087E-11 |
| m3/day | m3/s | | 1.1574074E-5 |
| m3/hr | m3/s | | 2.7777778E-4 |
| m3/min | m3/s | | 1.6666667E-2 |
| m3/s | m3/s | | 1. |
| m3/year | m3/s | | 3.1688087E-8 |
| Mft3/day | m3/s | 1000 cubic feet per day | 0.327741279E-3 |
| MMft3/day | m3/s | million cubic feet per day | 0.327741279 |
| MMft3/hr | m3/s | million cubic feet per hour | 7.8657907 |
| cm3/hr.K | m3/s.K | | 2.7777778E-10 |
| l/min.m | m3/s.m | | 1.6666667E-5 |
| l/s.m | m3/s.m | | 0.001 |
| m3/hr.m | m3/s.m | | 2.7777778E-4 |
| l/min.m2 | m3/s.m2 | | 1.6666667E-5 |
| l/s.m2 | m3/s.m2 | | 0.001 |
| m3/hr.m2 | m3/s.m2 | | 2.7777778E-4 |
| ft3/hr.psi | m3/s.Pa | | 1.140836E-9 |
| ft3/min.rpm | m3/s.rpm | | 4.7194744E-4 |
| ft3/s.rpm | m3/s.rpm | | 0.028316846 |
| gal/hr.rpm | m3/s.rpm | | 1.0515033E-6 |
| gal/min.rpm | m3/s.rpm | | 6.3090196E-5 |
| l/day.rpm | m3/s.rpm | | 1.157407E-8 |
| l/min.rpm | m3/s.rpm | | 1.6666667E-5 |
| l/s.rpm | m3/s.rpm | | 0.001 |
| m3/day.rpm | m3/s.rpm | | 1.1574074E-5 |
| m3/hr.rpm | m3/s.rpm | | 0.2777778E-3 |
| m3/s.rpm | m3/s.rpm | | 1. |
| m3/year.rpm | m3/s.rpm | | 3.1688087E-8 |
| ft3/s2 | m3/s2 | | 0.028316846 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|-------|---------|---------|---|
| m3/s2 | m3/s2 | | 1. |

| | | | |
|----------------|---------------|---|----------------|
| cm2.l/Ohm.mol2 | m5/Ohm.mol2 | square cm*liters per Ohm and mole squared | 1.E-7 |
| m5/Ohm.mol2 | m5/Ohm.mol2 | | 1. |
| cm2.l/s.mol | m5/s.mol | | 1.E-7 |
| m5/s.mol | m5/s.mol | | 1. |
| cm6/mol2 | m6/mol2 | | 1.E-12 |
| dm6/mol2 | m6/mol2 | | 1.E-6 |
| ft6/lbmol2 | m6/mol2 | | 3.8972502E-9 |
| l2/mol2 | m6/mol2 | | 1.E-6 |
| m6/mol2 | m6/mol2 | | 1. |
| cm9/mol3 | m9/mol3 | | 1.E-18 |
| dm9/mol3 | m9/mol3 | | 1.E-9 |
| ft9/lbmol3 | m9/mol3 | | 2.4329738E-13 |
| l3/mol3 | m9/mol3 | | 1.E-9 |
| m9/mol3 | m9/mol3 | | 1. |
| mass fraction | mass fraction | | 1. |
| kmol | mol | | 1000. |
| lbmol | mol | pound-mole | 453.592368 |
| mol | mol | | 1. |
| mol % | mol fraction | | 1.E-2 |
| mol fraction | mol fraction | | 1. |
| mol/mol | mol fraction | | 1. |
| kmol/cycle | mol/cycle | | 1000. |
| lbmol/cycle | mol/cycle | | 453.59237 |
| mol/cycle | mol/cycle | | 1.E-3 |
| lbmol/day | mol/day | | 5.249911667E-3 |
| lbmol/day.ft | mol/day.m | | 1.722412E-2 |
| mol/100g | mol/kg | | 10. |
| mol/kg | mol/kg | | 1. |
| molon | mol/kg | | 1. |
| umol/100 g | mol/kg | micro-mol per 100 grams | 1.E-5 |
| mol/m.min | mol/m.s | | 1.6666667E-2 |
| mol/m.s | mol/m.s | | 1. |
| dmol/m3 | mol/m3 | | 0.1 |
| kmol/m3 | mol/m3 | | 1.E3 |
| lbmol/ft3 | mol/m3 | | 1.6018463E4 |
| lbmol/gal | mol/m3 | | 1.1982643E5 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|-----------------|-----------------|---------|---|
| mmol/cm3 | mol/m3 | | 0.001 |
| mmol/l | mol/m3 | | 1. |
| mol/cm3 | mol/m3 | | 1.E6 |
| mol/dm3 | mol/m3 | | 1.E3 |
| mol/l | mol/m3 | | 1.E3 |
| mol/m3 | mol/m3 | | 1. |
| mol/l solvent | mol/m3 solvent | | 1000. |
| mol/m3 solvent | mol/m3 solvent | | 1. |
| mol/m3.K | mol/m3.K | | 1. |
| kmol/m3.atm | mol/m3.Pa | | 9.86923E-3 |
| mol/m3.atm | mol/m3.Pa | | 9.86923E-6 |
| mol/m3.Pa | mol/m3.Pa | | 1. |
| lbmol/ft3.hr | mol/m3.s | | 4.4495732 |
| lbmol/ft3.min | mol/m3.s | | 2.6697439E2 |
| lbmol/ft3.s | mol/m3.s | | 1.6018563E4 |
| mol/cm3.hr | mol/m3.s | | 3.6E9 |
| mol/cm3.s | mol/m3.s | | 1.E6 |
| mol/l.hr | mol/m3.s | | 0.277777778 |
| mol/l.s | mol/m3.s | | 1.E3 |
| mol/mol solvent | mol/mol solvent | | 1. |
| lbmol/atm.s | mol/Pa.s | | 0.0044766086 |
| lbmol/psi.min | mol/Pa.s | | 1.0964664E-3 |
| lbmol/psi.s | mol/Pa.s | | 6.5787985E-2 |
| mol/atm.hr | mol/Pa.s | | 2.7414535E-9 |
| mol/bar.hr | mol/Pa.s | | 2.7777778E-9 |
| mol/kPa.hr | mol/Pa.s | | 2.7777778E-7 |
| mol/kPa.min | mol/Pa.s | | 1.66666667E-5 |
| mol/kPa.s | mol/Pa.s | | 1.E-3 |
| kmol/day | mol/s | | 1.157407417E-5 |
| kmol/hr | mol/s | | 0.27777778 |
| kmol/s | mol/s | | 0.001 |
| lbmol/hr | mol/s | | 0.12599788 |
| lbmol/s | mol/s | | 0.45359237E3 |
| mol/min | mol/s | | 1.66666667E-2 |
| mol/s | mol/s | | 1.E-3 |
| kmol/day.m | mol/s.m | | 1.157407417E-5 |
| kmol/hr.m | mol/s.m | | 0.27777778E-6 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|--|--|---------|---|
| kmol/s.m | mol/s.m | | 0.001 |
| lbmol/hr.ft | mol/s.m | | 0.41337887 |
| lbmol/s.ft | mol/s.m | | 1.4881639E3 |
| kmol/hr.m ³ | mol/s.m ³ | | 0.27777778E-6 |
| kmol/s.m ³ | mol/s.m ³ | | 0.001 |
| kmol/hr.atm | mol/s.Pa | | 2.7414535E-6 |
| kmol/hr.bar | mol/s.Pa | | 2.77777778E-6 |
| kmol/hr.kPa | mol/s.Pa | | 2.77777778E-4 |
| kmol/hr.mmH ₂ O | mol/s.Pa | | 0.0283262437 |
| kmol/hr.Pa | mol/s.Pa | | 0.27777778 |
| kmol/min.kPa | mol/s.Pa | | 0.0166666667 |
| kmol/s.atm | mol/s.Pa | | 9.8692327E-9 |
| kmol/s.bar | mol/s.Pa | | 1.E-8 |
| kmol/s.kPa | mol/s.Pa | | 1.E-6 |
| mol-l | mol-l | | 1. |
| mol ² /l ² | mol ² /m ⁶ | | 1.E6 |
| mol ² /m ⁶ | mol ² /m ⁶ | | 1. |
| mol/100g solvent | molal | | 10. |
| mol/g solvent | molal | | 1000. |
| mol/kg solvent | molal | | 1. |
| molal | molal | | 1. |
| molal-l | molal-l | | 1. |
| molar | molar | | 1. |
| dyn | N | | 1.0E-5 |
| lb(force) | N | | 4.4482216 |
| N | N | | 1. |
| dyn ^(1/4) .cm ^(11/4) /ml | N ^(1/4) .m ^(11/4) /mol | | 1.7782794E-7 |
| N ^(1/4) .m ^(11/4) /mol | N ^(1/4) .m ^(11/4) /mol | | 1. |
| lb(force).ft | N.m | | 1.3558179 |
| lb(force).ft/lb | N.m/kg | | 2.989067 |
| lb(force).ft/s | N.m/s | | 1.3558179 |
| mN.s/m ² | N.s/m ² | | 0.001 |
| dyn/cm | N/m | | 1.E-3 |
| lb(force)/ft | N/m | | 14.593903 |
| mN/m | N/m | | 1.E-3 |
| N/m | N/m | | 1. |

| | | | |
|--------|-----|--|----|
| N/m2.m | N/m | | 1. |
|--------|-----|--|----|

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|---------------|-----------|------------------------------------|---|
| lb(force)/ft2 | N/m2 | | 47.880259 |
| lb(force)/ft3 | N/m3 | | 157.08747 |
| mmH2O/m | N/m3 | | 9.806348 |
| N/m3 | N/m3 | | 1. |
| Ohm | Ohm | | 1. |
| Ohm.cm | Ohm.m | | 0.01 |
| Ohm.m | Ohm.m | | 1. |
| Ohm-1 | Ohm-1 | | 1. |
| Ohm-1.cm-1 | Ohm-1.m-1 | | 100. |
| Ohm-1.m-1 | Ohm-1.m-1 | | 1. |
| Sie/cm | Ohm-1.m-1 | | 100. |
| Sie/m | Ohm-1.m-1 | | 1. |
| Ohm-1.m-3 | Ohm-1.m-3 | | 1. |
| Sie/ml | Ohm-1.m-3 | | 1.E6 |
| ata | Pa | absolute atmospheres | 98066.5 |
| atm | Pa | | 101325. |
| bar | Pa | | 1.E5 |
| cmH2O | Pa | cm of water column (pressure) | 98.063754 |
| Gpa | Pa | | 1.E9 |
| Hpa | Pa | | 100. |
| inH2O | Pa | inches of water columns (pressure) | 249.0889 |
| inHg(32F) | Pa | | 3386.39 |
| inHg(60F) | Pa | | 3332.69 |
| kbar | Pa | | 1.E8 |
| kg(force)/cm2 | Pa | | 98066.5 |
| kN/m2 | Pa | | 1000. |
| kp/cm2 | Pa | | 98066.5 |
| kp/m2 | Pa | | 9.80665 |
| kPa | Pa | | 1.E3 |
| lb(force)/in2 | Pa | | 6.89476E3 |
| lb/in2 | Pa | | 6.89476E3 |
| mbar | Pa | | 100. |
| mmH2O | Pa | mm of water column | 9.806348 |
| mmHg | Pa | mm of Hg column (Torr) | 133.3223684 |

| | | | |
|-------------------|----|--|-------|
| MN/m ² | Pa | | 1.E6 |
| mPa | Pa | | 1.E-3 |
| MPa | Pa | | 1.E6 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|--|---|------------------------|---|
| mTorr | Pa | | 0.1333224 |
| N/m ² | Pa | | 1. |
| Pa | Pa | | 1. |
| psi | Pa | pounds per square inch | 6894.7573 |
| Torr | Pa | | 133.3224 |
| ata.K | Pa.K | | 98066.5 |
| atm.K | Pa.K | | 101325. |
| kPa.K | Pa.K | | 1000. |
| Pa.K | Pa.K | | 1. |
| kg(force).m/kg | Pa.m/kg | | 9.80665 |
| bar.m/s | Pa.m/s | | 1.E5 |
| Pa.m/s | Pa.m/s | | 1. |
| atm.ft ³ /lbmol | Pa.m ³ /mol | | 6.3255133 |
| Pa.cm ³ /mol | Pa.m ³ /mol | | 1.E6 |
| Pa.dm ³ /mol | Pa.m ³ /mol | | 1.E3 |
| Pa.m ³ /mol | Pa.m ³ /mol | | 1. |
| psi.ft ⁶ | Pa.m ⁶ | | 5.5285184 |
| atm.dm ⁶ .K/mol ² | Pa.m ⁶ .K/mol ² | | 0.101325 |
| Pa.m ⁶ .K/mol ² | Pa.m ⁶ .K/mol ² | | 1. |
| atm.l ² .K ² /mol ² | Pa.m ⁶ .K ² /mol ² | | 0.101325 |
| bar.m ⁶ .K ² /mol ² | Pa.m ⁶ .K ² /mol ² | | 1.E5 |
| kPa.m ⁶ .K ² /mol ² | Pa.m ⁶ .K ² /mol ² | | 1000. |
| Pa.m ⁶ .K ² /mol ² | Pa.m ⁶ .K ² /mol ² | | 1. |
| bar.cm ⁶ /g.K | Pa.m ⁶ /kg.K | | 1.E2 |
| Pa.m ⁶ /kg.K | Pa.m ⁶ /kg.K | | 1. |
| atm.l ² /mol ² | Pa.m ⁶ /mol ² | | 0.101325 |
| kPa.m ⁶ /mol ² | Pa.m ⁶ /mol ² | | 1000. |
| Pa.m ⁶ /mol ² | Pa.m ⁶ /mol ² | | 1. |
| psi.ft ⁶ /lbmol ² | Pa.m ⁶ /mol ² | | 2.68706E-5 |
| psi.ft ⁹ | Pa.m ⁹ | | 0.15655021 |
| kPa.m ⁹ .K ² /mol ³ | Pa.m ⁹ .K ² /mol ³ | | 1000. |
| kPa.m ⁹ /mol ³ | Pa.m ⁹ /mol ³ | | 1000. |
| Pa.m ⁹ /mol ³ | Pa.m ⁹ /mol ³ | | 1. |

| | | | |
|----------------|-------------|------------|--------------|
| psi.ft9/lbmol3 | Pa.m9/mol3 | | 1.6774764E-9 |
| kbar.mol.K/cm3 | Pa.mol.K/m3 | | 1.E14 |
| Pa.mol.k/m3 | Pa.mol.K/m3 | | 1. |
| cP | Pa.s | centipoise | 0.001 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|-------------------|-------------------|------------------------|---|
| g/cm.s | Pa.s | | 0.1 |
| kg(force).s/m2 | Pa.s | | 9.80665 |
| kg/m.s | Pa.s | | 1. |
| kp.s/m2 | Pa.s | | 9.807 |
| lb(force).s/ft2 | Pa.s | | 47.880262 |
| lb/ft.hr | Pa.s | | 4.1337887E-4 |
| lb/ft.s | Pa.s | | 1.48816 |
| mP | Pa.s | | 1.E-4 |
| mPa.s | Pa.s | | 1.E-3 |
| N.s/m2 | Pa.s | | 1. |
| P | Pa.s | | 0.1 |
| Pa.s | Pa.s | | 1. |
| psi.hr | Pa.s | | 2.4821136E7 |
| ug/cm.s | Pa.s | mico-gram per cm and s | 1.E-7 |
| uP | Pa.s | micropoise | 1.E-7 |
| uPa.s | Pa.s | micro-Pascal-seconds | 1.E-6 |
| mPa.s.cm3/g | Pa.s.m3/kg | | 1.E-6 |
| Pa.s.m3/kg | Pa.s.m3/kg | | 1. |
| uPa.s.cm3/g | Pa.s.m3/kg | micro-Pascal.s.cm3/g | 1.E3 |
| Pa.s/K | Pa.s/K | | 1. |
| Pa.s/K2 | Pa.s/K2 | | 1. |
| Pa.s/K3 | Pa.s/K3 | | 1. |
| cP/mol % | Pa.s/mol fraction | | 0.1 |
| cP/mol fraction | Pa.s/mol fraction | | 0.001 |
| Pa.s/mol fraction | Pa.s/mol fraction | | 1. |
| lb/ft.hr2 | Pa.s2 | | 1.1482746E-7 |
| lb/ft.s2 | Pa.s2 | | 1.4881662 |
| ata/K | Pa/K | | 98066.5 |
| atm/K | Pa/K | | 101325. |
| bar/K | Pa/K | | 1.E5 |
| kbar/K | Pa/K | | 1.E8 |
| kPa/K | Pa/K | | 1.E3 |

| | | | |
|--------|------|--|-----------|
| mbar/K | Pa/K | | 1.E2 |
| mPa/K | Pa/K | | 1.E-3 |
| MPa/K | Pa/K | | 1.E6 |
| Pa/K | Pa/K | | 1. |
| psi/F | Pa/K | | 12410.568 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|-------------------|-----------------|---------|---|
| Torr/K | Pa/K | | 133.3224 |
| ata/m | Pa/m | | 98066.5 |
| atm/m | Pa/m | | 101325. |
| bar/km | Pa/m | | 100. |
| bar/m | Pa/m | | 1.E5 |
| cmH2O/m | Pa/m | | 98.063754 |
| inH2O/ft | Pa/m | | 817.2208 |
| inHg(32F)/ft | Pa/m | | 11110.203 |
| kPa/km | Pa/m | | 1.E6 |
| kPa/mm | Pa/m | | 1. |
| mbar/m | Pa/m | | 1.E2 |
| mH2O/m | Pa/m | | 98.063754 |
| mmHg/ft | Pa/m | | 437.4094 |
| Pa/m | Pa/m | | 1. |
| psi/100ft | Pa/m | | 2.2620595E2 |
| psi/ft | Pa/m | | 2.2620595E4 |
| Torr/ft | Pa/m | | 437.40945 |
| kbar/cm3.mol | Pa/m3.mol | | 1.E14 |
| Pa/m3.mol | Pa/m3.mol | | 1. |
| ata/mol fraction | Pa/mol fraction | | 98066.5 |
| atm/mol fraction | Pa/mol fraction | | 101325. |
| bar/mol fraction | Pa/mol fraction | | 1.E5 |
| kPa/mol fraction | Pa/mol fraction | | 1.E3 |
| MPa/mol fraction | Pa/mol fraction | | 1.E6 |
| Pa/(mol/mol) | Pa/mol fraction | | 1. |
| Pa/mol fraction | Pa/mol fraction | | 1. |
| psi/mol fraction | Pa/mol fraction | | 6894.76 |
| Torr/mol fraction | Pa/mol fraction | | 133.3224 |
| ata/s | Pa/s | | 98066.5 |
| atm/s | Pa/s | | 101325. |
| bar/s | Pa/s | | 1.E5 |

| | | | |
|---------------------|--------------------|--|------------|
| Pa/s | Pa/s | | 1. |
| atm/weight fraction | Pa/weight fraction | | 101325. |
| Pa/weight fraction | Pa/weight fraction | | 1. |
| MPa^0.5 | Pa^0.5 | | 1.E3 |
| Pa^0.5 | Pa^0.5 | | 1. |
| ata-1 | Pa-1 | | 1.01972E-5 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|---------------|----------|---------|---|
| atm-1 | Pa-1 | | 9.86923E-6 |
| bar-1 | Pa-1 | | 1.E-5 |
| cm2/dyn | Pa-1 | | 10. |
| cm2/kg(force) | Pa-1 | | 1.0197162E-5 |
| cm2/kp | Pa-1 | | 1.01972E-5 |
| Gpa-1 | Pa-1 | | 1.E-9 |
| inH2O-1 | Pa-1 | | 4.0146309E-3 |
| kbar-1 | Pa-1 | | 1.E-8 |
| kPa-1 | Pa-1 | | 1.E-3 |
| m2/kp | Pa-1 | | 0.101972 |
| m2/N | Pa-1 | | 1. |
| mbar-1 | Pa-1 | | 1.E-2 |
| mmH2O-1 | Pa-1 | | 0.1019748 |
| mPa-1 | Pa-1 | | 1.E3 |
| MPa-1 | Pa-1 | | 1.E-6 |
| Pa-1 | Pa-1 | | 1. |
| psi-1 | Pa-1 | | 1.4503774E-4 |
| Torr-1 | Pa-1 | | 7.500615E-3 |
| TPa-1 | Pa-1 | | 1.E-12 |
| atm-1.K-1 | Pa-1.K-1 | | 9.86923E-6 |
| Pa-1.K-1 | Pa-1.K-1 | | 1. |
| P-1 | Pa-1.s-1 | | 10. |
| Pa-1.s-1 | Pa-1.s-1 | | 1. |
| ata-2 | Pa-2 | | 1.0398289E-10 |
| atm-2 | Pa-2 | | 9.7401753E-11 |
| bar-2 | Pa-2 | | 1.E-10 |
| kPa-2 | Pa-2 | | 1.E-6 |
| mbar-2 | Pa-2 | | 1.E-4 |
| Pa-2 | Pa-2 | | 1. |
| Torr-2 | Pa-2 | | 5.6259226E-5 |

| | | | |
|--------|------|--|---------------|
| ata-3 | Pa-3 | | 1.0603225E-15 |
| atm-3 | Pa-3 | | 9.6128057E-16 |
| bar-3 | Pa-3 | | 1.E-15 |
| kPa-3 | Pa-3 | | 1.E-9 |
| mbar-3 | Pa-3 | | 1.E-6 |
| Pa-3 | Pa-3 | | 1. |
| Torr-3 | Pa-3 | | 4.219788E-7 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|----------------|----------|--------------|---|
| ata-4 | Pa-4 | | 1.081228E-20 |
| atm-4 | Pa-4 | | 9.4871016E-21 |
| bar-4 | Pa-4 | | 1.E-20 |
| kPa-4 | Pa-4 | | 1.E-12 |
| mbar-4 | Pa-4 | | 1.E-8 |
| Pa-4 | Pa-4 | | 1. |
| Torr-4 | Pa-4 | | 3.1651005E-9 |
| day | s | | 86400. |
| hr | s | | 3600. |
| min | s | | 60. |
| ms | s | | 0.001 |
| ns | s | | 1.E-9 |
| ps | s | | 1.E-12 |
| s | s | | 1. |
| us | s | microseconds | 0.000001 |
| year | s | | 31536000. |
| hr.ft2.Rnk/BTU | s.m2.K/J | | 1.7611019E-1 |
| hr.m2.K/kcal | s.m2.K/J | | 8.5984523E-1 |
| s.cm2.K/cal | s.m2.K/J | | 2.3884590E-5 |
| s.m2.K/J | s.m2.K/J | | 1.0 |
| s.m2.K/kcal | s.m2.K/J | | 2.3884590E-4 |
| s.m2.K/kJ | s.m2.K/J | | 1.0E-3 |
| day-1 | s-1 | | 1.1574074E-5 |
| GHz | s-1 | | 1.E9 |
| kHz | s-1 | | 1000. |
| MHz | s-1 | | 1000000. |
| rad/s | s-1 | | 0.15915475 |
| year-1 | s-1 | | 3.1688088E-8 |
| kV | V | | 1.E3 |

| | | | |
|------------|-----------------|--|-------|
| mV | V | | 1.E-3 |
| V | V | | 1. |
| V/cm | V/m | | 100. |
| V/m | V/m | | 1. |
| val/kg | val/kg | | 1. |
| val/l | val/m3 | | 1.E3 |
| val/m3 | val/m3 | | 1. |
| cm3/100cm3 | volume fraction | | 0.01 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|--------------------|-----------------|--------------|---|
| cm3/cm3 | volume fraction | | 1. |
| cm3/l | volume fraction | | 1.E-3 |
| l/m3 | volume fraction | | 1.E-3 |
| m3/m3 | volume fraction | | 1. |
| ml/m3 | volume fraction | | 1.E-6 |
| volume % | volume fraction | | 0.01 |
| volume fraction | volume fraction | | 1. |
| BTU/s | W | | 1.0550559E3 |
| erg/s | W | | 1.E-7 |
| hp | W | hourse power | 745.69987 |
| kcal/s | W | | 4.1868E3 |
| kp.m/s | W | | 9.80665 |
| kW | W | | 1000. |
| PS | W | | 745.700 |
| W | W | | 1. |
| hp.hr | W.s | | 2.6845195E6 |
| kW/cycle | W/cycle | | 1000. |
| W/cycle | W/cycle | | 1. |
| W/degC | W/K | | 1 |
| W/K | W/K | | 1. |
| W/kg | W/kg | | 1. |
| W/m | W/m | | 1. |
| BTU.in/ft2.hr.degF | W/m.K | | 0.14422789 |
| BTU.in/ft2.hr.Rnk | W/m.K | | 0.14422789 |
| BTU/ft.hr.degF | W/m.K | | 1.7307347 |
| BTU/ft.s.degF | W/m.K | | 6230.6449 |
| BTU/in.hr.degF | W/m.K | | 20.768816 |
| BTU/in.s.degF | W/m.K | | 7.4767738E4 |

| | | | |
|----------------|-------|--|-----------|
| cal/cm.s.K | W/m.K | | 4.1868E2 |
| cal/km.s.K | W/m.K | | 4.1868E-3 |
| cal/m.hr.K | W/m.K | | 1.163E-3 |
| cal/m.s.K | W/m.K | | 4.1868 |
| erg/cm.s.K | W/m.K | | 1.E-5 |
| J/cm.s.K | W/m.K | | 1.E2 |
| J/m.s.K | W/m.K | | 1. |
| kcal.m/hr.m2.K | W/m.K | | 1.163 |
| kcal/m.hr.K | W/m.K | | 1.163 |

| unit | SI-unit | remarks | factor unit -> SI-unit (only for information) |
|-------------|-----------------|-------------------------|---|
| kcal/m.s.K | W/m.K | | 4.1868E3 |
| kW/m.K | W/m.K | | 1.0E3 |
| mW/cm.degC | W/m.K | | 0.1 |
| mW/cm.K | W/m.K | | 0.1 |
| mW/m.K | W/m.K | | 0.001 |
| uW/cm.K | W/m.K | micro-Watt per cm and K | 0.0001 |
| W/cm.K | W/m.K | | 1.E2 |
| W/m.K | W/m.K | | 1. |
| W/m.K2 | W/m.K2 | | 1. |
| W/m.K3 | W/m.K3 | | 1. |
| W/m.K4 | W/m.K4 | | 1. |
| W/m2 | W/m2 | | 1 |
| cal/cm2.s.K | W/m2.K | | 4.1868E4 |
| kW/m2.K | W/m2.K | | 1.0E3 |
| W/m2.degC | W/m2.K | | 1. |
| W/m2.K | W/m2.K | | 1. |
| W/m2.s.K | W/m2.s.K | | 1. |
| hp/ft3 | W/m3 | | 2.6334143E4 |
| kW/l | W/m3 | | 1.E6 |
| kW/m3 | W/m3 | | 1.E3 |
| W/m3 | W/m3 | | 1. |
| W/mol | W/mol | | 1. |
| hp/lbmol.hr | W/mol.s | | 4.566631EE-4 |
| hp/lbmol.s | W/mol.s | | 1.64398709 |
| kW/kmol.hr | W/mol.s | | 2.7777778E-4 |
| kW/kmol.s | W/mol.s | | 1. |
| g/100g | weight fraction | | 1.E-2 |

| | | | |
|-----------------|-----------------|--|-------|
| g/g | weight fraction | | 1. |
| g/kg | weight fraction | | 0.001 |
| kg/kg | weight fraction | | 1. |
| mg/kg | weight fraction | | 1.E-6 |
| ppm | weight fraction | | 1.E-6 |
| weight % | weight fraction | | 1.E-2 |
| weight fraction | weight fraction | | 1. |

bbl = petroleum barrel, USA (42 US liquid gallons)

cal(th) = thermochemical calory

gal = liquid gallons, USA hp =

mechanical horse power lb = pound

(avdp.) oz = ounces (avdp.) u... =

mikro... m... = milli... M... = Mega...

6.1.3. Pure Component Constant Properties (CAPE-OPEN)

7 Schedule

| | Step 1 | Step 2 | Step 3 | Step 4 | Step 5 | Step 6 |
|-----------------------------|--|---------------------|-------------------|---------------------|------------------------|--------|
| User Interface | Graphical Drag & Drop User Interface | | | | | |
| | Stream and Unit Operations Input Forms | | | | | |
| Units Converter | Basic Unit Conversions, T, P, Q, etc | | | | | |
| Basic Thermo | Component Database | Low Level Functions | Equation of State | Flash Calculations | Distillation Algorithm | |
| | Pure | PSat1 | | Bubble & Dew Points | | |
| | Binary | CPIG | | Isothermal Flash | | |
| | Viscosity Database | HVIG | | Constant H Flash | | |
| | Thermal Conductivity | SVIG | | Constant S Flash | | |
| | Surface Tension | CPIGMX | | | | |
| | | HVIGMX | | | | |
| | | SVIGMX | | | | |
| Transport Properties | | Visc_L, Visc_V | | | | |
| | | K_L, K_V | | | | |

| | | | | | | |
|--|--|-------|--|--|--|---|
| | | Sigma | | | | |
| Reactors | | | | | Stoichiometric | |
| | | | | | Rate Based | |
| | | | | | Equilibrium | |
| Other Unit Operations | | | | | Splitters | |
| | | | | | Mixers Component Separator | |
| Equipment Sizing | | | | | Lines Drums/Vessels Trays Heat Exchangers | |
| | | | | | | |
| | | | | | | |
| Report Generation | | | | | Stream Report Unit Operations Report Other Reports | |
| | | | | | | |
| Kernel Development | | | | | | Sequencing & Solving |
| Flowsheet Specifications & Optimization | | | | | | Controllers, Adjust Blocks, Design-Spec, Optimizers |

8 Structure Description

- I. Global Variables: The following variables are GLOBAL. They are defined in the mdlThermoControl module

| Variable | Description | Type | Units |
|----------|----------------------|---------|-------|
| N_Comp | Number of Components | Integer | --- |
| T | Temperature | Double | K |
| P | Pressure | Double | Bar |
| Vfrac | Vapor Fraction | Double | --- |

| | | | |
|------|-------------------------------|--------|-----------|
| ZL | Liquid Compressibility Factor | Double | --- |
| ZV | Vapor Compressibility Factor | Double | --- |
| HLMX | Liquid Molar Enthalpy | Double | J/gmole |
| HVMX | Vapor Molar Enthalpy | Double | J/gmole |
| HMX | Mixture Molar Enthalpy | Double | J/gmole |
| SLMX | Liquid Molar Entropy | Double | J/gmole.K |
| SVMX | Vapor Molar Enthalpy | Double | J/gmole.K |
| SMX | Mixture Molar Enthalpy | Double | J/gmole.K |
| Z() | Overall Mole Fraction | Double | --- |
| Y() | Vapor Mole Fraction | Double | --- |
| X() | Liquid Mole Fraction | Double | --- |

II. Equations of State

Every equation of state should be in a separate module. All subroutines and functions that related to the EOS should be PRIVATE (not accessible to other routines) except for the ones listed below. If the name of the equation of state is ABC, then the equation should have the following subroutines

| Routine | Description | Arguments |
|---------|------------------------|----------------------|
| ABCZMX | Compressibility Factor | T, P, X(), N, IPhase |
| ABCPHX | Fugacity Coefficients | Phi, T, P, X(), N, Z |
| ABCHDM | Enthalpy Departure | T, P, Z, X(), N |

| | | |
|--------|-------------------|-----------------|
| ABCHDM | Entropy Departure | T, P, Z, X(), N |
|--------|-------------------|-----------------|

Where

T, P and N are the temperature, pressure and number of components respectively.

I_{Phase} = 0 is to call for a liquid compressibility factor

I_{Phase} = 1 is to call for a vapor compressibility factor

X() containing the compositions

Z: Compressibility factor

Phi: Array for fugacity coefficients.

III. Streams

The streams are currently work in progress and will be modified as needed. The initial thinking is to define the streams in a Pascal “Record” so that the stream properties can be access as follows:

Stream(1).Temp. Stream(1).Pres, etc.

The following are the parameters stored in a stream record

| Parameter | Description | Type |
|-------------|---|--------|
| Tag | Stream Tag | String |
| Name | Stream Name | String |
| Source | The operation the stream is coming from | |
| Destination | The operation the steam is going to | |
| Temp | Temperature | Double |

| | | |
|----------|--|---------|
| Pres | Pressure | Double |
| Vfrac | Vapor Fraction | Double |
| ZL | Liquid Compressibility Factor | Double |
| ZV | Vapor Compressibility Factor | Double |
| HLMX | Liquid Molar Enthalpy | Double |
| HVMX | Vapor Molar Enthalpy | Double |
| HMX | Mixture Molar Enthalpy | Double |
| SLMX | Liquid Molar Entropy | Double |
| SVMX | Vapor Molar Enthalpy | Double |
| SMX | Mixture Molar Enthalpy | Double |
| Z() | Overall Mole Fraction | Double |
| Y() | Vapor Mole Fraction | Double |
| X() | Liquid Mole Fraction | Double |
| ZM() | Overall Mass Fraction | Double |
| MW | Molecular Weight | Double |
| Flow | Molar Flow Rate | Double |
| MassFlow | Mass Flow Rate | Double |
| Has_Flow | Indicates if the steam has a flow rate | Boolean |
| Has_Comp | Indicates if the steam has composition | Boolean |
| Has_Temp | Indicates if the steam has Temperature | Boolean |
| Has_Pres | Indicates if the steam has Pressure | Boolean |

| | | |
|-----------|---|---------|
| Has_Vfrac | Indicates if the steam has Vapor Fraction | Boolean |
| Has_HMX | Indicates if the steam has Enthalpy | Boolean |
| IsSolved | Indicates if the stream is Solved | Boolean |

IV. Units

The units are set by the pure component database I will be donating. The reference pressure for heats of formation and Gibbs free energy of formation in this database is 1 bar, same for heat capacity. The following is a list of all key units that will be used in the heart of the simulator. User entries should be converted to these units (e.g. steam temperature, pressure, etc) BEFORE they are stored in the appropriate location.

| Property | Units |
|-----------------|-----------|
| Temperature | K |
| Pressure | Bar |
| Molar Flow Rate | gmole/hr |
| Mass Flow Rate | grams/hr |
| Enthalpy | J/gmole |
| Entropy | J/gmole.K |
| Heat Duty/Power | J/hr |

I agree, this is the most disgusting set of units I have ever seen but let's put up with it for now.

V.
VI.