

MANUALES DE ASPENONE. TERMODINÁMICA

Este documento describe la creación de un nuevo archivo, la selección de componentes, la selección de la ecuación de estado y métodos de convergencia.

DGAPA / PAPIME / PEI 103325

CREACIÓN DE
UN ARCHIVO
NUEVO

Creación de un Archivo Nuevo

Este documento describe la creación de un nuevo proyecto en Aspen Plus en la versión 12.1. Para este ejemplo se seleccionan tres componentes presentes en la base de datos y se muestran diferentes formas de como buscarlos en la pestaña de selección:

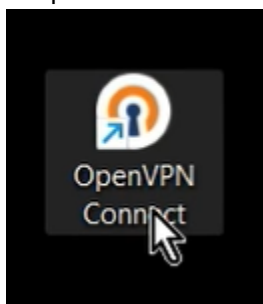
Componente
Dióxido de Carbono
Estireno
Divinil Benceno

El siguiente procedimiento está ampliamente descrito en un video al final de este documento. Se insertan videos que describen menús desplegables y casillas de selección.

Procedimiento

El video que a continuación se muestra abarca los siguientes puntos:

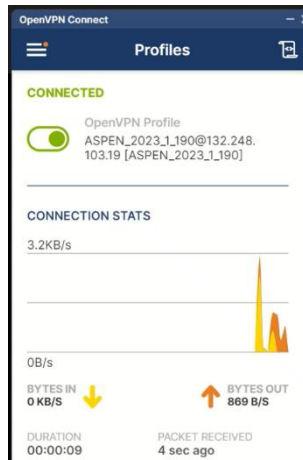
- 1) Inicio de sesión de ASPEN.
 - a. Abrir aplicación VPN. Esto conectará el dispositivo con el servidor de la Facultad de Química.



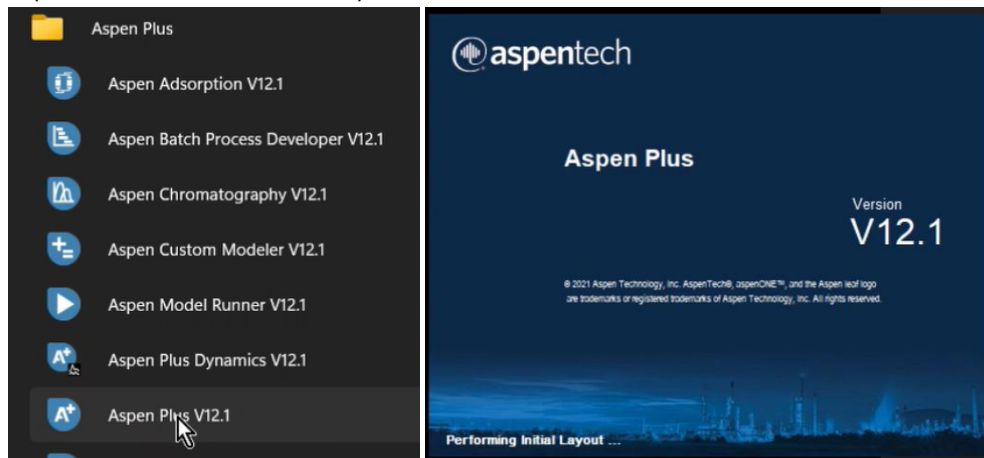
- b. Al dar abrir el ícono, se abrirá una ventana donde se muestra un interruptor.



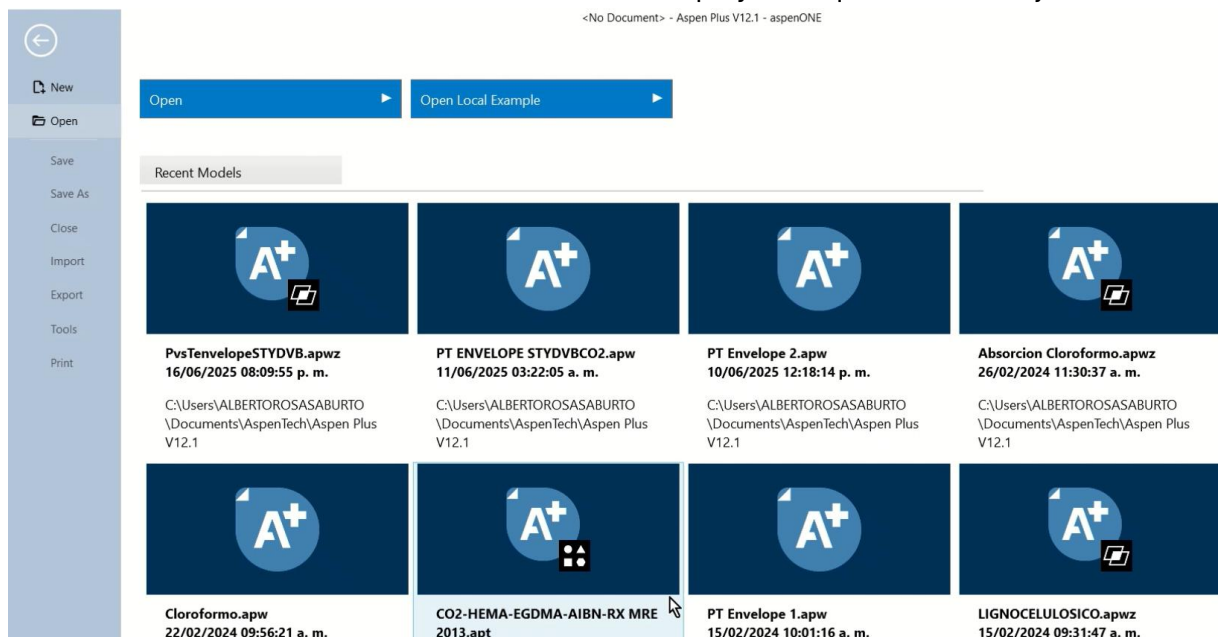
- c. Una vez activado el interruptor se observará que el dispositivo entra en comunicación con el servidor de la Facultad de Química.



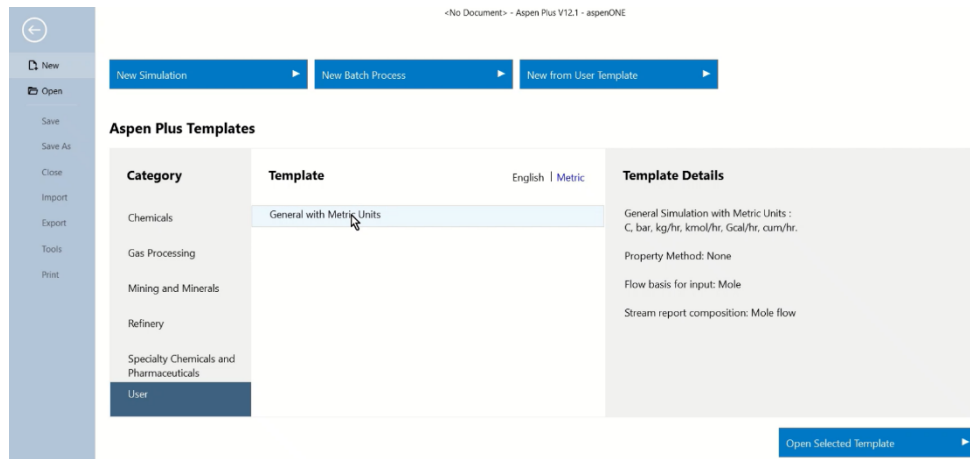
- d. Una vez que el dispositivo se conectó con el servidor de la Facultad de Química, se procede a abrir ASPEN Plus (en este caso versión 12.1).



- e. Al abrir ASPENONE se observa un menú con los últimos proyectos que se han trabajado.

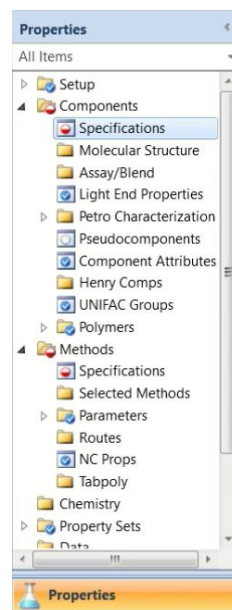


- 2) Crear un archivo nuevo, seleccionándolo de distintos formatos.
- En este ejemplo se crea un archivo nuevo:



b. En el video se muestran diferentes partes de ASPENONE:

i. Módulo de propiedades:



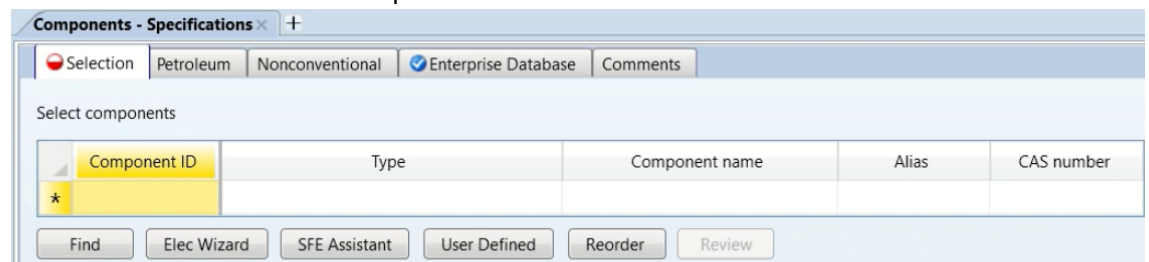
ii. Cada sección para llenar o incompleta se muestra como una media luna roja y blanca.



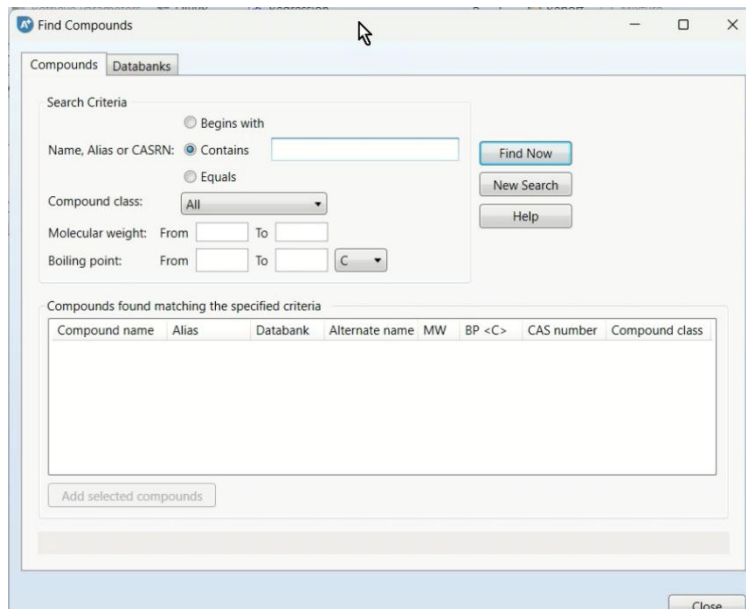
iii. Lo primero por llenar es el listado de los componentes:



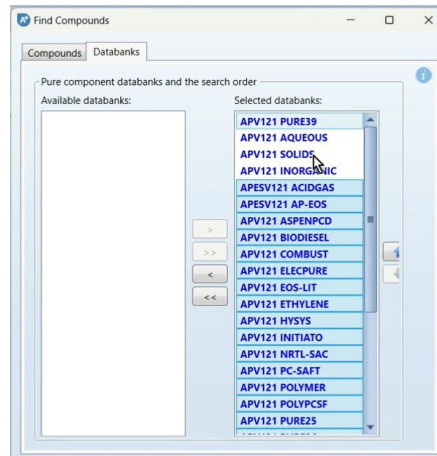
iv. Al seleccionar este menú de "Specifications" se observa una tabla:



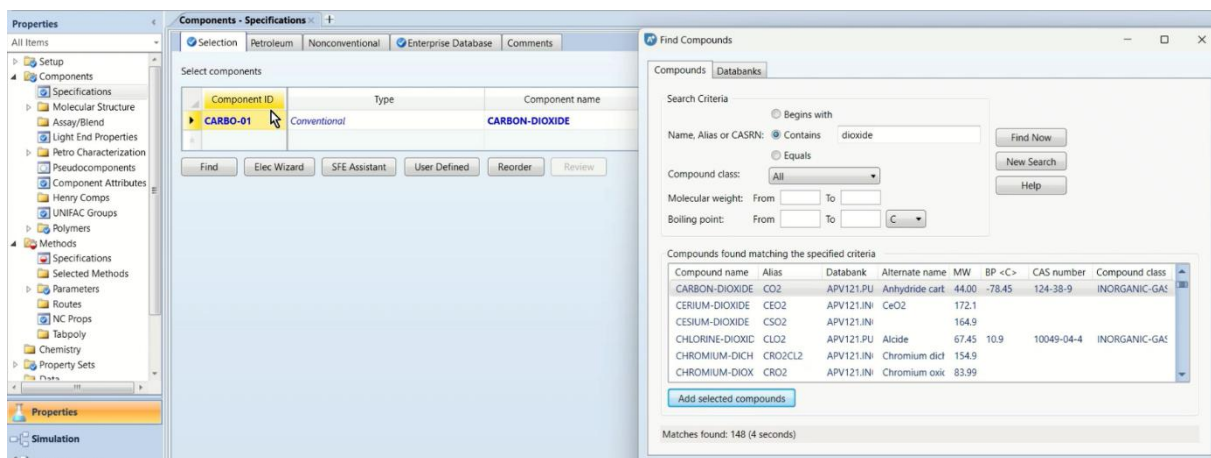
v. En esta tabla se deben ir llenando con los componentes a emplear. Para ello se deberá seleccionar el botón "Find". Esto despliega un menú emergente:



- vi. En este menú seleccionamos la pestaña “Databanks”. En esta pestaña elegimos las bases de datos a emplear seleccionándolas y pasándolas de la columna “Available databanks” hacia “Selected databanks” con las flechas botón.



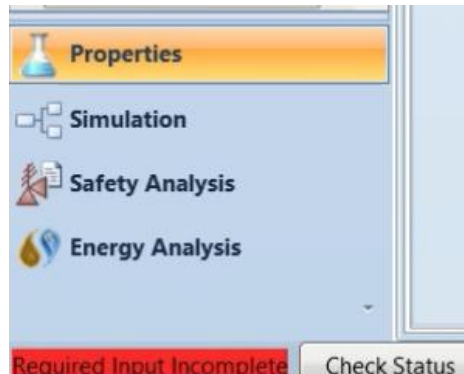
- vii. Regresamos a la pestaña “Compounds” para buscar los componentes.
viii. En dicho menú buscamos por las diferentes opciones de búsqueda el componente deseado y lo agregamos a la lista de componentes.



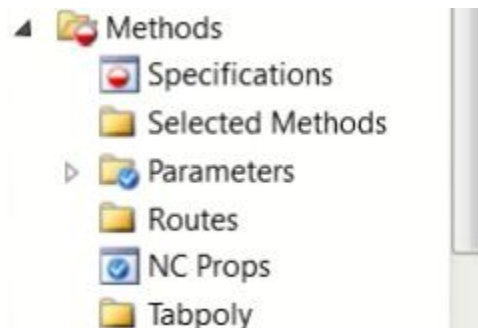
- ix. Repetir la búsqueda de componentes hasta completar la lista.

Components - Specifications				
Selection Petroleum Nonconventional Enterprise Database Comments				
Select components				
Component ID	Type	Component name	Alias	CAS number
CARBO-01	Conventional	CARBON-DIOXIDE	CO2	124-38-9
STYRE-01	Conventional	STYRENE	C8H8	100-42-5
1:4-D-01	Conventional	1,4-DIETHENYLBENZENE	C10H10-N1	105-06-6
Find Elec Wizard SFE Assistant User Defined Reorder Review				

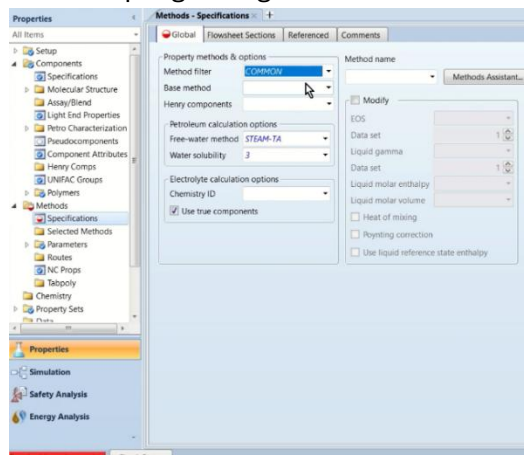
- 3) En la parte inferior izquierda sigue apareciendo en rojo en el estatus del proceso “Required input incompleted”.



- a. Para completar la primera parte es necesario ahora establecer las ecuaciones de estado y tipo de cálculo para este proceso. Esto se hace en el menú de “Properties” en la carpeta de “Methods”, en la aplicación “Specifications”.

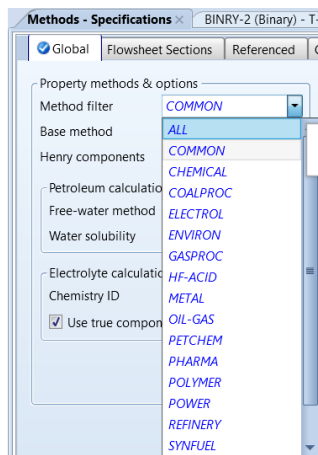


- b. Al seleccionar “Specifications” se despliega el siguiente menú:



- c. En la pestaña de “Methods-Specifications” se observan diferentes casillas a llenar:
- Method filter: Es un filtro para reducir la lista de ecuaciones de estado en la lista desplegable “Base Method”. Este filtro reduce el número de ecuaciones de estado a desplegar según la

aplicación o proceso a simular. Si no se elige ningún proceso el valor predeterminado que se muestra es “COMMON” (selección de ecuaciones más comunes). Si se desea ver todo el catálogo de ecuaciones de estado se selecciona “ALL”.



- ii. Base method: Define la ecuación de estado a usar. A continuación mostramos en el menú desplegable cada cartel emergente con su explicación:

Base method: AMINES Henry components: Kent-Eisenberg model for Amines systems.	Base method: APISOUR Henry components: API sour water method.
Base method: B-PITZER Henry components: Bromley-Pitzer model for aqueous electrolyte systems.	Base method: BK10 Henry components: Braun K-10 property method for petroleum applications.
Base method: BWR-LS Henry components: BWR Lee-Starling equation of state.	Base method: BWRS Henry components: Benedict-Webb-Rubin-Starling equation of state.
Base method: CHAO-SEA Henry components: Chao-Seader correlation with Lee-Kesler enthalpy.	Base method: COSMOSAC Henry components: COSMO-SAC with Ideal gas and Henry's law.
Base method: CPA Henry components: Cubic-Plus-Association EOS Package.	Base method: ELECRTL Henry components: Electrolyte NRTL model with Redlich-Kwong equation of state. For aqueous and mixed solvent applications.
Base method: ENRTL-HF Henry components: Electrolyte NRTL model with HF equation of state. For mixed solvent applications.	Base method: ENRTL-HG Henry components: Electrolyte NRTL model with Redlich-Kwong equation of state. Uses Helgeson model for equilibrium constants estimation and for standard properties.
Base method: ENRTL-RK Henry components: Unsymmetric electrolyte NRTL model with Redlich-Kwong equation of state and Henry's law for electrolyte systems under unsymmetric reference state for ionic species.	Base method: ENRTL-SR Henry components: Symmetric electrolyte NRTL model with Redlich-Kwong equation of state and Henry's law for electrolyte systems under symmetric reference state for all components.
Base method: EPNRTL Henry components: Electrolyte-Polymer NRTL model with Redlich-Kwong equation of state. For aqueous and mixed solvent applications including polymers.	Base method: FACT Henry components: FACT property method to be used with the Aspen/FACT/ChemApp interface. This method requires an external ChemSage data file and ChemApp license.
Base method: GERG2008 Henry components: GERG 2008 model for properties of natural gas systems.	Base method: GPSWAT Henry components: GPA sour water method based on the GPA Sour Water Equilibria Correlation and Computer Program (GPA RR-118).
Base method: GRAYSON Henry components: Grayson-Streed correlation with Lee-Kesler enthalpy.	Base method: GRAYSON2 Henry components: Grayson-Streed with enthalpy of water calculated from NBS steam tables.
Base method: HANSEN Henry components: Hansen with Ideal gas and Henry's law.	Base method: HYSGLYCO Henry components: HYSYS Glycol EOS package.
Base method: HYSR Henry components: HYSYS Peng-Robinson EOS package.	Base method: HYSSRK Henry components: HYSYS Soave-Redlich-Kwong EOS package.
Base method: IAPWS-95 Henry components: IAPWS formulation 1995 for the Thermodynamic properties of water. This is the current standard of International Association for the Properties of Water and Steam.	Base method: IDEAL Henry components: Ideal property method. Uses both Raoult's law and Henry's law.
Base method: IP97 Henry components: IAPWS Industrial Formulation 1997 correlation for thermodynamic properties of water and steam. More computationally efficient than the IAPWS 1995 scientific formulation.	Base method: LK-PLOCK Henry components: Lee-Kesler-Plocker equation of state.
Base method: MXBONNEL Henry components: Maxwell-Bonnel model. Should be used with STMB52 property method for the free-water phase.	Base method: NRTL Henry components: NRTL (Renon) with Ideal gas and Henry's law.
Base method: NRTL-2 Henry components: NRTL (Renon) with Ideal gas and Henry's law. Uses second set of binary parameters.	Base method: NRTL-HOC Henry components: NRTL (Renon)/Hayden-O'Connell equation of state with Henry's law.
Base method: NRTL-NTH Henry components: NRTL (Renon)/Nothnagel equation of state with Henry's law.	Base method: NRTL-RK Henry components: NRTL (Renon)/Redlich-Kwong equation of state with Henry's law.
Base method: NRTL-SAC Henry components: NRTL-SAC with Ideal gas and Henry's law.	Base method: OLI Henry components: OLI property method for electrolytes applications. Required special license from OLI Systems Inc.

Base method **PC-SAFT**
Henry components
Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) property method for copolymer systems

Base method **PITZ-HG**
Henry components
Pitzer model for aqueous electrolyte systems. Uses Helgeson model for equilibrium constants estimation and for standard properties.

Base method **PNRTL-IG**
Henry components
Polymer NRTL model with ideal gas law.

Base method **POLYNRTL**
Henry components
Polymer-NRTL/Redlich-Kwong equation of state with Henry's law for polymers simulation.

Base method **POLYSAFT**
Henry components
Statistical Associating Fluid Theory (SAFT) property method for polymers simulation.

Base method **POLYSRK**
Henry components
Predictive Redlich-Kwong-Soave equation of state for polymers simulation.

Base method **POLYUFV**
Henry components
UNIFAC free volume/Redlich-Kwong equation of state with Henry's law for polymers simulation.

Base method **PR-BM**
Henry components
Peng-Robinson equation of state with Boston-Mathias modifications.

Base method **PRWS**
Henry components
Peng-Robinson equation of state with Wong-Sandler mixing rules.

Base method **REFPROP**
Henry components
REFPROP model (NIST Reference Fluid Thermodynamic and Transport Properties) for refrigerants, hydrocarbons, and natural gas systems.

Base method **RK-SOAVE**
Henry components
Redlich-Kwong-Soave equation of state.

Base method **RKSMHV2**
Henry components
Redlich-Kwong-Soave equation of state with modified Huron-Vidal mixing rules.

Base method **RTOMXB**
Henry components
Maxwell-Bonnell model. Should be used with RTOSTM property method for the free-water phase. For upward compatibility with RT-OPT only.

Base method **RTOSTM**
Henry components
NBS/NRC steam tables. Recommended for use with the RTOMXB, RTOSRK property methods. For upward compatibility with RT-OPT only.

Base method **SRK-ML**
Henry components
Soave-Redlich-Kwong equation of state with T-dependent k_{ij} . $U_{ij} = k_{ij} - k_{ij}$, option to calculate enthalpy of water from NBS steam tables

Base method **SOLIDS**
Henry components
Property method for general solids and pyrometallurgy applications.

Base method **STEAM-TA**
Henry components
ASME 1967 steam table correlations.

Base method **STMNBS2**
Henry components
NBS/NRC steam tables. Recommended for use with the BWRS, MXBONNELL, GRAYSON2 property methods. The same equations as STEAMNBS, but with different root search method.

Base method **UNIF-DMD**
Henry components
Dortmund modified UNIFAC.

Base method **UNIF-LBY**
Henry components
Lynby modified UNIFAC.

Base method **UNIFAC**
Henry components
UNIFAC with Redlich-Kwong equation of state and Henry's law.

Base method **UNIQ-HOC**
Henry components
UNIQUAC/Hayden-O'Connell equation of state with Henry's law.

Base method **UNIQ-RK**
Henry components
UNIQUAC/Redlich-Kwong equation of state with Henry's law.

Base method **VANL-2**
Henry components
Van Laar with Ideal gas and Henry's law. Uses second set of binary parameters.

Base method **VANL-NTH**
Henry components
Van Laar/Nothnagel equation of state with Henry's law.

Base method **VANLAAR**
Henry components
Van Laar with Ideal gas and Henry's law.

Base method **WILS-2**
Henry components
Wilson with Ideal gas and Henry's law. Uses second set of binary parameters.

Base method **WILS-HF**
Henry components
Wilson/HF equation of state with Henry's law.

Base method **PENG-ROB**
Henry components
Peng-Robinson equation of state.

Base method **PITZER**
Henry components
Pitzer model for aqueous electrolyte systems.

Base method **POLYFH**
Henry components
Flory-Huggins/Redlich-Kwong equation of state with Henry's law for polymers simulation.

Base method **POLYPCSF**
Henry components
Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) property method for polymers simulation.

Base method **POLYSL**
Henry components
Sanchez-Lacombe property method for polymers simulation.

Base method **POLYUF**
Henry components
UNIFAC/Redlich-Kwong equation of state with Henry's law for polymers simulation.

Base method **PPR78**
Henry components
PPR78 EOS (predictive 1978, Peng-Robinson EOS with temperature dependent KJ) calculated through a group contribution method.

Base method **PRMHV2**
Henry components
Peng-Robinson equation of state with modified Huron-Vidal mixing rules.

Base method **PSRK**
Henry components
Predictive Redlich-Kwong-Soave equation of state.

Base method **RK-ASPEN**
Henry components
Redlich-Kwong-Aspen equation of state.

Base method **RKS-BM**
Henry components
Redlich-Kwong-Soave equation of state with Boston-Mathias modifications.

Base method **RKSW**
Henry components
Redlich-Kwong-Soave equation of state with Wong-Sandler mixing rules.

Base method **RTOSRK**
Henry components
Soave-Redlich-Kwong equation of state model (PML implementation). Should be used with RTOSTM property method for the free-water phase. For upward compatibility with RT-OPT only.

Base method **SRK**
Henry components
Soave-Redlich-Kwong equation of state with T-dependent k_{ij} , option to calculate enthalpy of water from NBS steam tables, and composition-independent fugacity coefficients option.

Base method **SRKDD**
Henry components
Soave-Redlich-Kwong equation of state with Kabadi-Danner modifications for water-hydrocarbon systems. See SRK property method for other features.

Base method **SR-POLAR**
Henry components
Schwartzentruber-Renon equation of state for highly non-ideal systems.

Base method **STEAMNBS**
Henry components
NBS/NRC steam tables.

Base method **SYSOP0**
Henry components
Ideal/Raoult's Law.

Base method **UNIF-HOC**
Henry components
UNIFAC/Hayden-O'Connell equation of state with Henry's law.

Base method **UNIF-LL**
Henry components
UNIFAC for liquid-liquid systems with Redlich-Kwong equation of state and Henry's law.

Base method **UNIQ-2**
Henry components
UNIQUAC with Ideal gas and Henry's law. Uses second set of binary parameters.

Base method **UNIQ-NTH**
Henry components
UNIQUAC/Nothnagel equation of state with Henry's law.

Base method **UNIQUAC**
Henry components
UNIQUAC with Ideal gas and Henry's law.

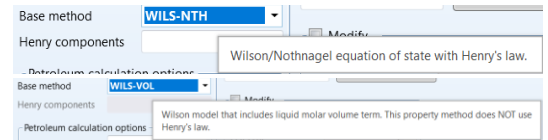
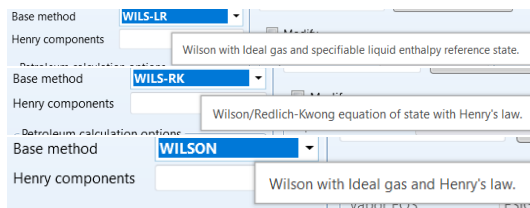
Base method **VANL-HOC**
Henry components
Van Laar/Hayden-O'Connell equation of state with Henry's law.

Base method **VANL-RK**
Henry components
Van Laar/Redlich-Kwong equation of state with Henry's law.

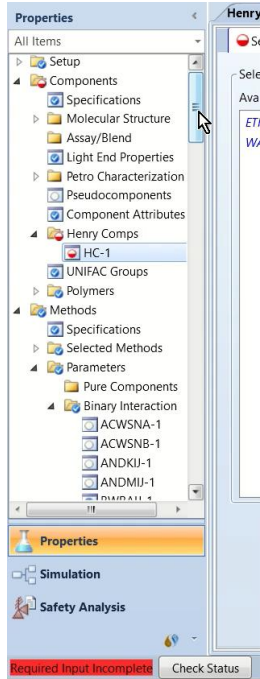
Base method **VTPR**
Henry components
Volume-Translated Peng-Robinson EOS Package.

Base method **WILS-GLR**
Henry components
Wilson with Ideal gas EOS and specifiable ideal-gas/liquid enthalpy reference states.

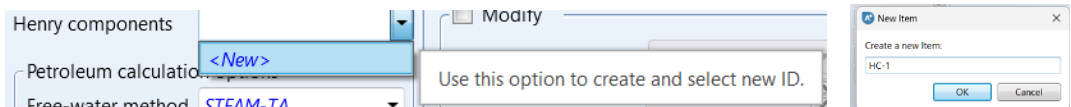
Base method **WILS-HOC**
Henry components
Wilson/Hayden-O'Connell equation of state with Henry's law.



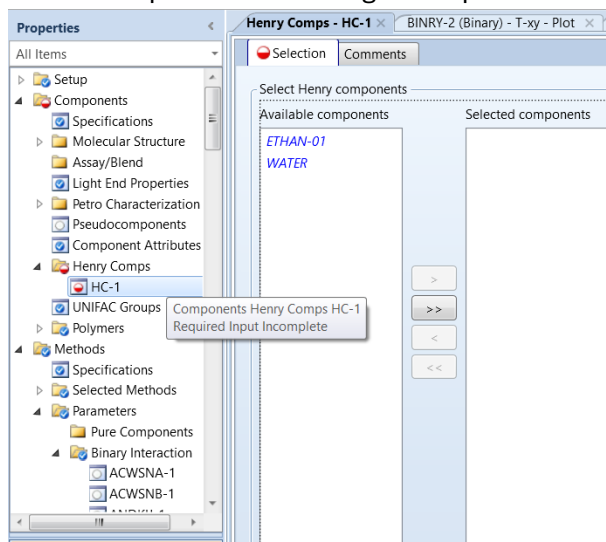
- iii. Cada vez que se seleccione una ecuación de estado en el menú “Properties” aparecerá en la carpeta de “Parameters\Binary Interaction” aparecerán aplicaciones donde se estimarán o se solicitarán valores para distintos parámetros de interacción.



- iv. En la selección “Henry components” se adicionan componentes a través de una ventana emergente. En diferentes modelos esta opción no se habilita o se deja en blanco.



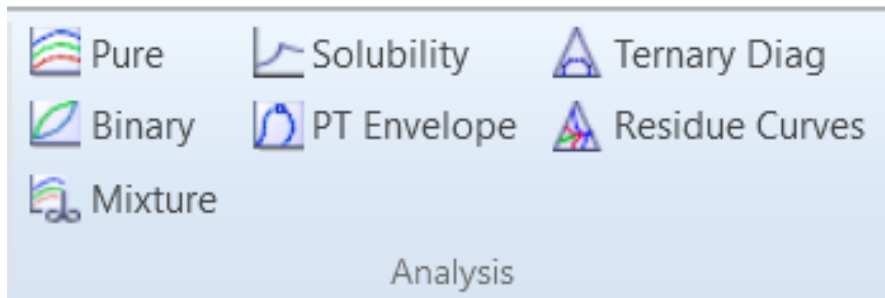
- v. Si se selecciona la opción de crear un grupo de componentes que sigan el modelo de Henry se deben de seleccionar los componentes en la siguiente pestaña.



- vi. Una vez seleccionados los componentes, la ecuación de estado y que se han revisado o llenado los campos de los parámetros y coeficientes binarios, se observará el siguiente letrero en la parte inferior izquierda: “Required Properties Input Complete”.

Required Properties Input Complete Check Status

- vii. Una vez que se tiene completada esta parte se procede a seleccionar el tipo de cálculo termodinámico a realizar en el submenú “Analysis”. En el menú “File” hay una sección en la parte superior derecha donde se puede seleccionar el tipo de cálculo:



Referencias:

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7. Medeiros, M. (2024). *Equilibrio de Fases y Químico* (2nd ed.). Facultad de Química, UNAM.

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INCORPORACION DE TIC'S PARA LA ENSEÑANZA Y EVALUACION DEL DESEMPEÑO DE LOS ALUMNOS EN ASIGNATURAS COMPARTIDAS DE DOS CARRERAS DE LA FACULTAD DE QUIMICA.

