

PPSC Gas Properties Calculator

User Manual

September 2026



PPSC Gas Properties
Calculator Software

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Overview

The PPSC Gas Properties Calculator is an engineering software developed to calculate and visualize thermophysical properties of pure gases and gas mixtures over a wide range of pressure and temperature conditions. The software provides a simple interface for engineers, researchers, and students to quickly evaluate gas behavior for petroleum, natural gas, CCUS, geothermal, acid gas, and other energy applications.

Users can select a pure component or create a user-defined gas mixture by specifying individual components and their mole fractions. Pressure and temperature can be entered using different engineering units. For pure components, the software interpolates or extrapolates laboratory data from the National Institute of Standards and Technology (NIST) to determine fluid properties at a specified pressure and temperature. For gas mixtures, the software uses reliable engineering correlations and calculation methods to estimate key properties, including molecular weight, compressibility factor (Z-factor), density, viscosity, phase, gas specific gravity, liquid specific gravity, and pseudo-critical pressure and temperature.

In addition to calculations at a single operating condition, the software provides advanced visualization and sensitivity-analysis tools. Users can generate property maps over pressure-temperature ranges, including density and viscosity surface maps, Z-factor maps, phase maps, isotherm curves, and sensitivity-gradient maps. These tools help users understand how gas properties change with pressure and temperature and identify regions where fluid properties are particularly sensitive to operating conditions.

Overall, the PPSC Gas Properties Calculator combines gas-property calculations, phase evaluation, visualization, and sensitivity analysis in one easy-to-use engineering platform.

Main Window

The main window of the PPSC Gas Properties Calculator provides a simple interface for entering operating conditions, defining fluid composition, performing property calculations, and reviewing the calculated results. Users can specify the pressure and temperature and select the appropriate engineering units for each input. When the user-defined mixture mode is selected, the Mixture Builder allows users to add or remove individual gas components and enter the mole fraction of each component. The software automatically calculates and displays the total mole fraction as the composition is being entered. To ensure that the mixture composition is physically valid, the sum of all component mole fractions must equal exactly 1.00 before the calculation can be performed. If the total is different from 1.00, the software will display a warning and prevent the prediction from proceeding until the composition is corrected. Once all required inputs are properly entered, the user can click Predict to calculate the gas properties, which are then displayed in the results panel on the right side of the main window.

PPSC Gas Properties Calculator
Pure components from tables • Mixtures from correlation model

Mode Mixture (User-defined) **Sensitivity Analysis** **Plot Maps** **Predict**

Pressure 1500.0 psia **Temperature** 100.0 °F

Mixture Builder (mole fractions)

Add component CH₄ (Methane) **Add** **Remove** **Sum: 1.000000**

Component	Mole fraction
CH ₄ (Methane)	0.970000
C ₂ H ₆ (Ethane)	0.020000
N ₂ (Nitrogen)	0.010000

Property **Value**

Note: For supercritical states, Gas Specific Gravity is referenced to air at the same pressure and temperature, while Liquid Specific Gravity is referenced to water at the same pressure and temperature.

Figure 1. Main calculator window before Predict is run.

Select the Calculation Mode

Use the Mode drop-down menu to select the fluid to be evaluated. The menu includes Mixture (User-defined) and available pure components such as CO₂, H₂S, N₂, C₂H₆, C₃H₈, and CH₄. Select Mixture (User-defined) when the fluid contains more than one component.

PPSC Gas Properties Calculator
Pure components from tables • Mixtures from correlation model

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Pressure Mixture (User-defined) **Temperature** 100.0 °F

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Property **Value**

Note: For supercritical states, Gas Specific Gravity is referenced to air at the same pressure and temperature, while Liquid Specific Gravity is referenced to water at the same pressure and temperature.

Figure 2. Mode selection menu.

Define Working Conditions

Enter the operating pressure and temperature in the input boxes near the top of the calculator. The units can also be changed using the unit selectors beside each value. Always confirm both the numerical value and its unit before running the calculation.

Pressure: enter the desired operating pressure and select the appropriate pressure unit.

Temperature: enter the desired operating temperature and select the appropriate temperature unit.

When units are changed, verify that the displayed operating condition represents the intended physical condition.

Build a User-Defined Mixture

When Mixture (User-defined) is selected, use the Mixture Builder to define the composition. Choose a component from the Add component drop-down menu and click Add. To delete a component, select it in the mixture list and click Remove. Enter the mole fraction for each component.

The Sum indicator shows the total mole fraction. A valid mixture requires a total of 1.000000. For example, the illustrated mixture contains 0.970 CH₄, 0.020 C₂H₆, and 0.010 N₂, giving a total of 1.000.

Predictions / Results

After the mode, operating conditions, and composition are correct, click Predict. The calculated properties appear in the results panel on the right.

The screenshot displays the PPSC Gas Properties Calculator interface. The top section shows the Mode set to 'Mixture (User-defined)', Pressure at 1500.0 psia, and Temperature at 100.0 °F. The Mixture Builder (mole fractions) section on the left lists three components: CH₄ (Methane) with a mole fraction of 0.970000, C₂H₆ (Ethane) with 0.020000, and N₂ (Nitrogen) with 0.010000. The total sum is 1.000000. The Results panel on the right displays various properties and their values:

Property	Value	Units
MW _{mix}	16.4432	lbm/lbmol
Z	0.856216	-
Phase	supercritical	-
Density	4.79622	lbm/ft ³
Gas Specific Gravity	N/A	-
Liquid Specific Gravity	0.0770204	-
Viscosity	0.0146082	cP
T _{pc}	-113.696	°F
P _{pc}	665.469	psia
T _{pc,corrected}	-113.696	°F
P _{pc,corrected}	665.469	psia
Temperature	100	°F

Note: For supercritical states, Gas Specific Gravity is referenced to air at the same pressure and temperature, while Liquid Specific Gravity is referenced to water at the same pressure and temperature.

Figure 3. Results displayed after clicking Predict.

Calculated outputs

Output	Meaning
MW_mix	Mixture molecular weight, representing the mole-fraction-weighted molecular mass of the mixture.
Z	Gas compressibility factor. Z indicates deviation from ideal-gas behavior; $Z = 1$ corresponds to ideal-gas behavior.
Phase	Predicted thermodynamic phase at the specified pressure, temperature, and composition, such as gas/vapor, liquid, two-phase, or supercritical.
Density	Fluid mass per unit volume at the specified operating condition.
Gas Specific Gravity	Relative gas density referenced to air. The program may report N/A when the state is not treated as a conventional gas state.
Liquid Specific Gravity	Relative liquid density referenced to water at the same pressure and temperature, as indicated by the software note.
Viscosity	Dynamic viscosity of the fluid, reported in the selected/displayed viscosity unit.
Tpc	Pseudo-critical temperature estimated for the mixture.
Ppc	Pseudo-critical pressure estimated for the mixture.
Tpc_corrected	Corrected pseudo-critical temperature when a correction is applied by the model.
Ppc_corrected	Corrected pseudo-critical pressure when a correction is applied by the model.
Temperature	The temperature used for the reported calculation.

Important: the software note states that for supercritical states, Gas Specific Gravity is referenced to air at the same pressure and temperature, while Liquid Specific Gravity is referenced to water at the same pressure and temperature. Interpret these values in the context of the predicted phase.

Plot Maps

Click Plot Maps from the main calculator to open the plotting interface. The Plot settings bar allows you to choose the Mode, Mixture, Property, and Chart type. After making the selections, click Plot to generate the visualization.

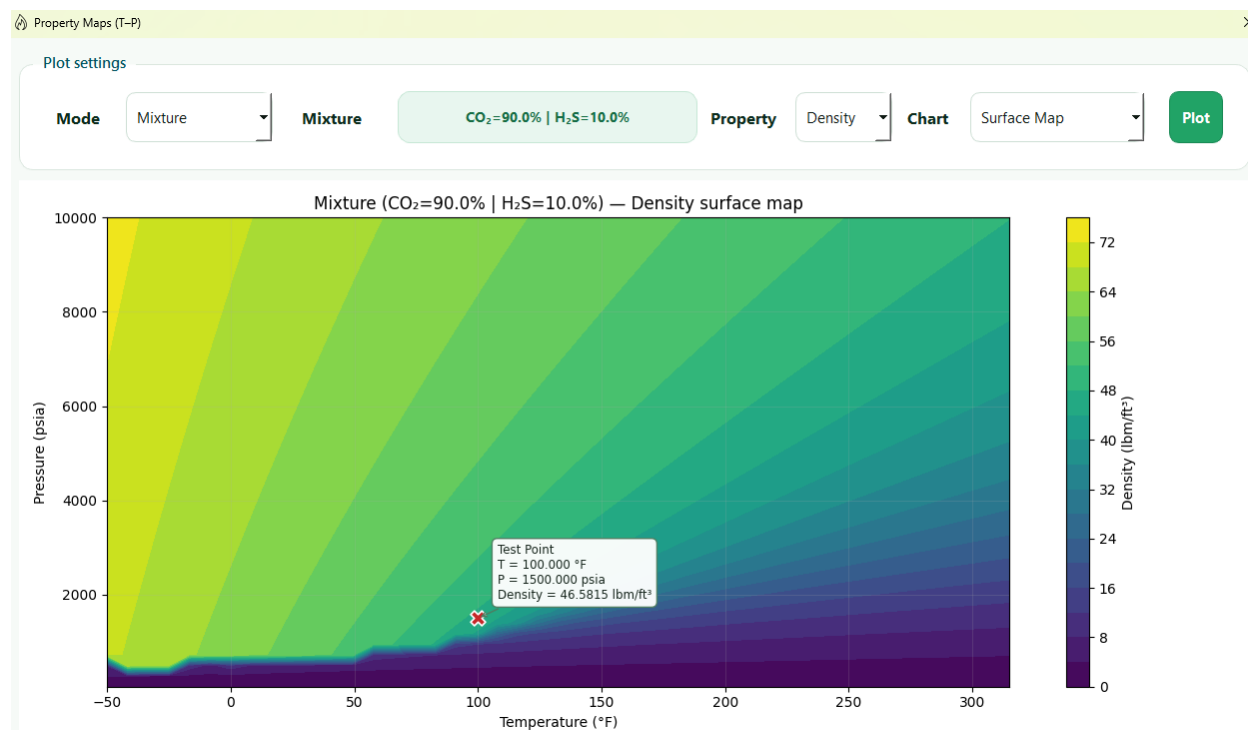


Figure 4. Density surface map for a 90% CO₂ / 10% H₂S mixture.

Plot settings

Mode: choose Pure component or Mixture.

Mixture: displays the selected mixture composition when Mixture mode is used.

Property: choose the property to visualize. Examples shown include Density, Viscosity, Z factor, and Phase.

Chart: choose the visualization type available for the selected property.

Plot: generates or refreshes the selected map or curve.

Surface Maps

A surface map displays how a selected property varies over the pressure-temperature space. Temperature is shown on the horizontal axis, pressure on the vertical axis, and the color scale represents the property magnitude. The marked Test Point identifies the current calculator operating condition and reports the corresponding value.

For the viscosity surface map, the color bar is viscosity in cP. For the density surface map, the color bar is density in lbm/ft³ in the illustrated configuration.

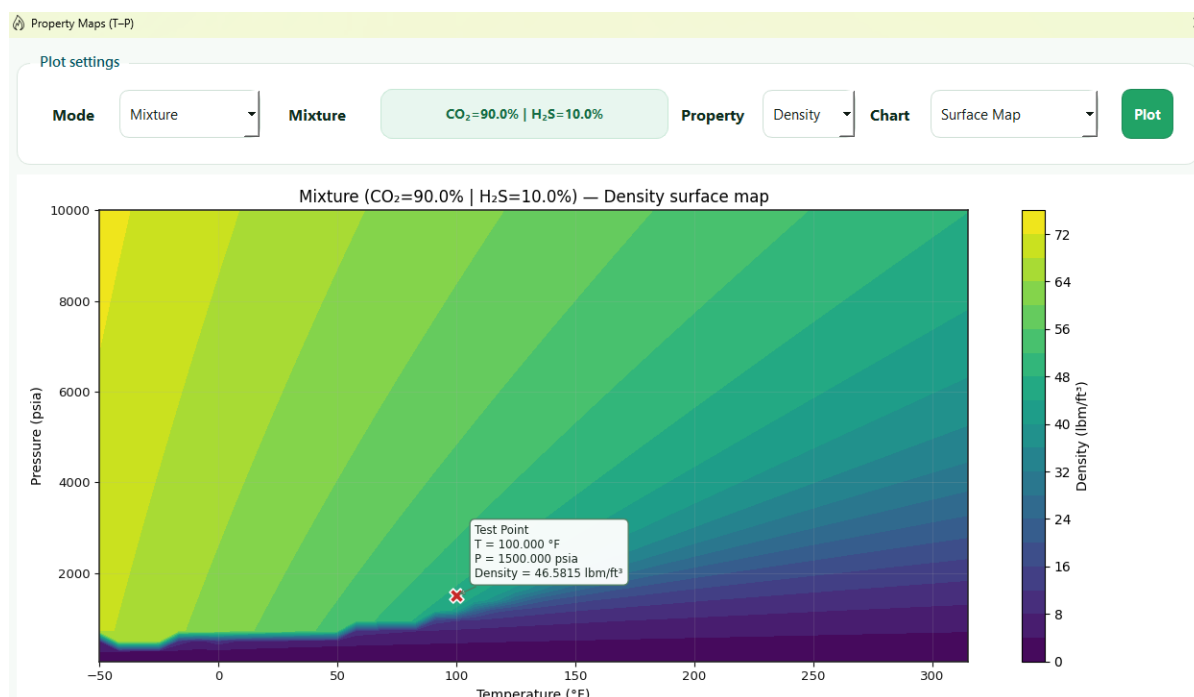


Figure 5. Density surface map for a 90% CO₂ / 10% H₂S mixture.

Isotherm Curves

Select Isotherm Curves to view the property as a function of pressure at fixed temperatures. A temperature line can be entered and added manually, or Auto can be used to generate representative temperature lines. The plot helps compare pressure dependence at several temperatures and can also display the current test point and pseudo-critical reference.

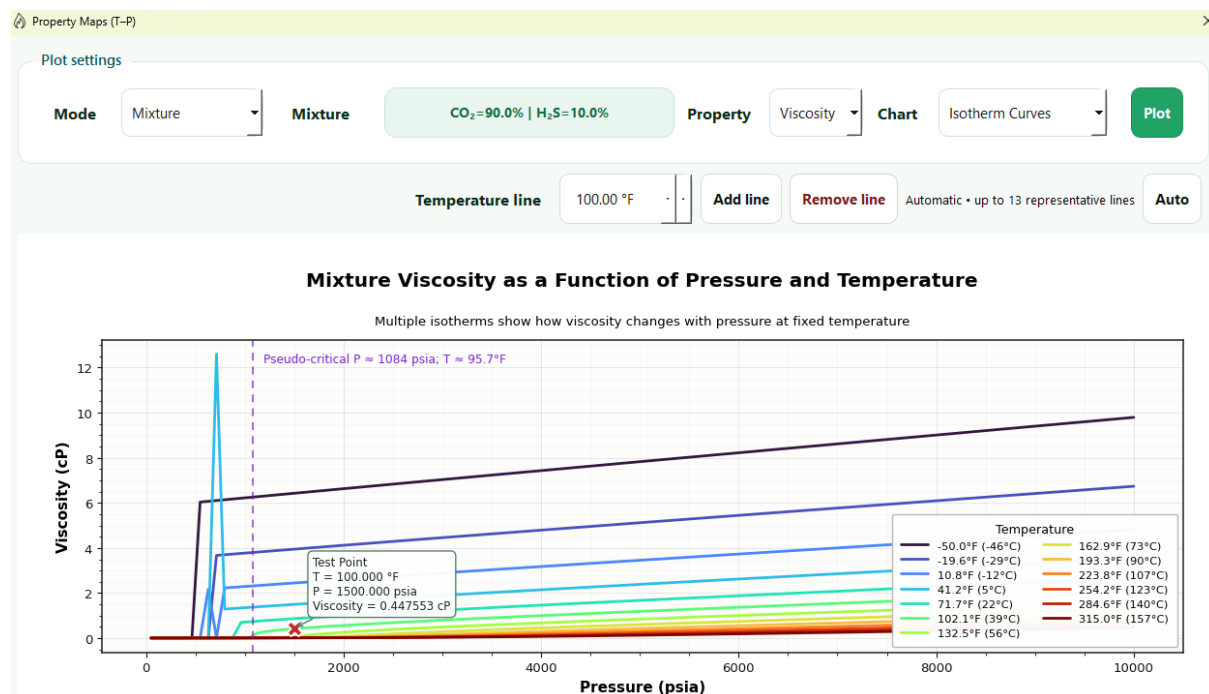


Figure 6. Viscosity isotherm curves for a 90% CO₂ / 10% H₂S mixture.

Sensitivity Gradient Map

The Sensitivity Gradient chart highlights regions where small changes in pressure or temperature produce the strongest local response in the selected property. Higher sensitivity-index values indicate greater local sensitivity. The display can identify the highest-sensitivity region and indicate whether pressure or temperature is the dominant local driver.

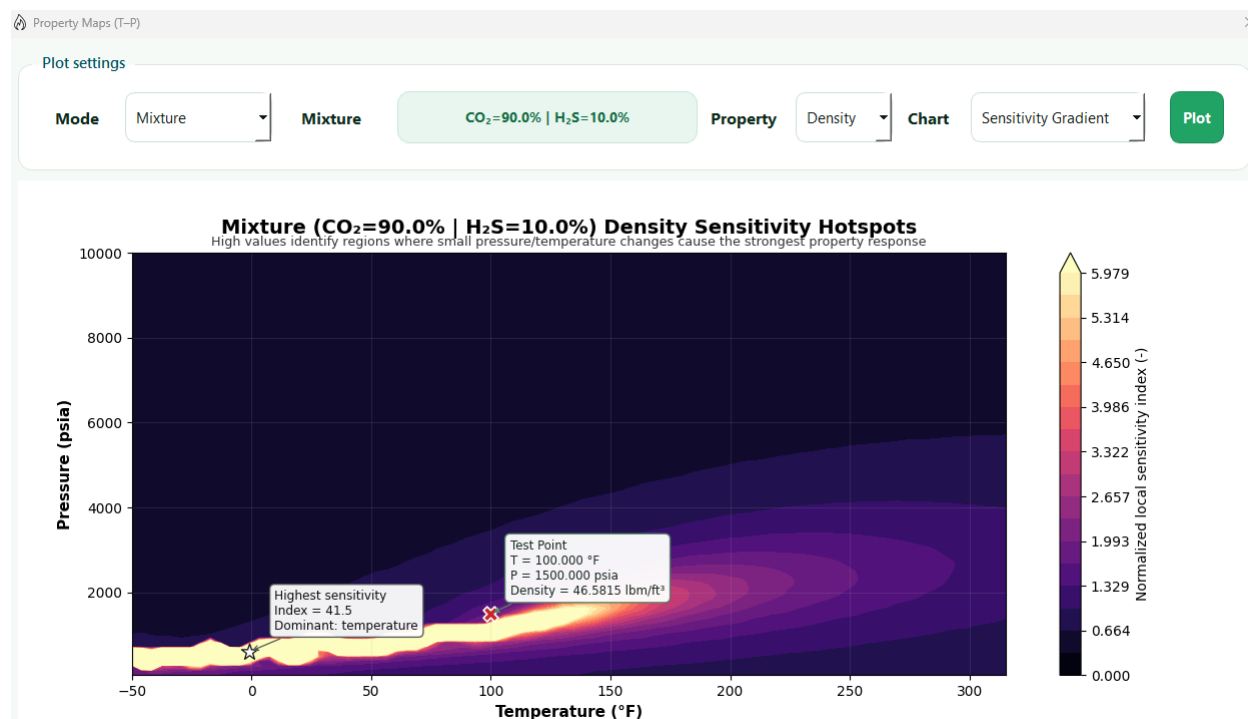


Figure 7. Density sensitivity-gradient map for a 90% CO₂ / 10% H₂S mixture.

Sensitivity Analysis

Click Sensitivity Analysis from the main calculator to evaluate the selected mixture over a user-defined pressure and temperature envelope. This tool calculates multiple cases and displays the response surface together with summary statistics and a table of calculated cases.

Define the analysis range

In Analysis Setup, specify the low value, high value, and step size for pressure and temperature. The Estimated Grid indicates the expected number of pressure points, temperature points, and cases. Click Run Sensitivity to perform the calculations.

Review sensitivity results

After the run is complete, the Response Surface shows the selected metric across the specified pressure-temperature range. Use the Metric selector to change the property being displayed. The summary boxes report the number of calculated cases and the minimum, average, and maximum values for the selected metric.

The Calculated Cases table provides the individual pressure-temperature cases and associated outputs such as Z factor, density, viscosity, and phase. Use Export Results to CSV when the calculated cases need to be saved for additional analysis or reporting.

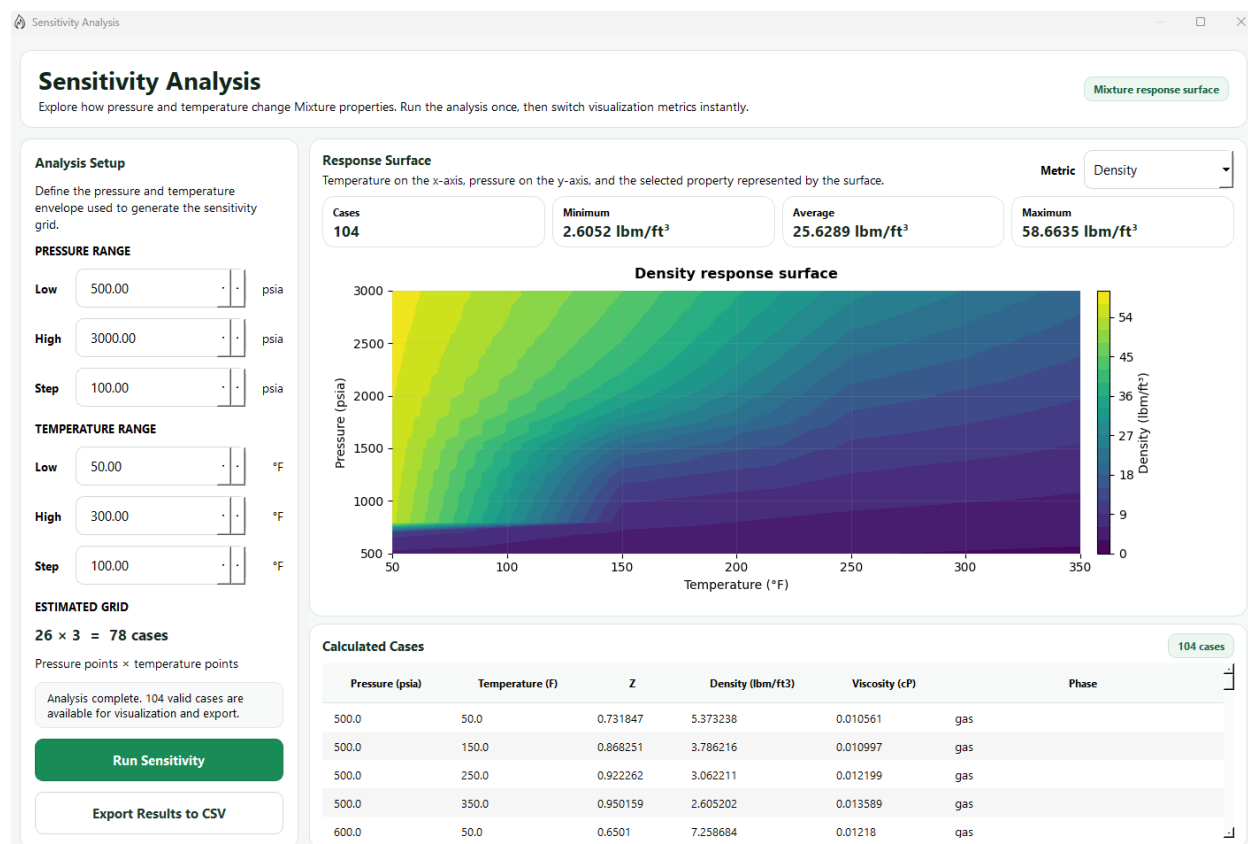


Figure 8. Sensitivity analysis window.

Contact

For more information, technical support, or inquiries about the PPSC Gas Properties Calculator Software, please contact us:

Website: <https://ppscnm.com>

Email: ppsc@ppscnm.com

Our team is available to assist with questions, software demonstrations, and technical support.