

CHO. A program to calculate fluid volumes, fugacities and activities in the Carbon–Hydrogen–Oxygen system.

Introduction

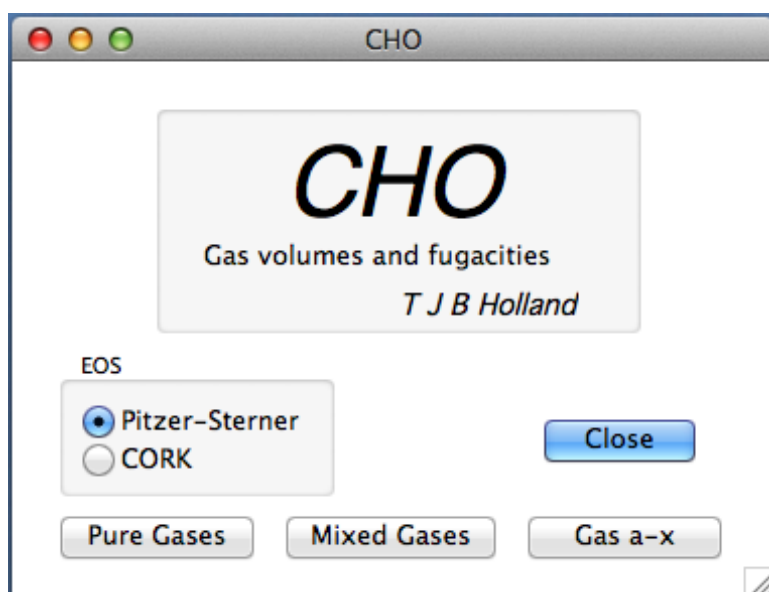
CHO is a program that uses the CORK equation of state (Holland & Powell 1991, *CMP* 109, 265–273) for fluids to calculate the following:

1. Volumes or fugacities of individual gas species (H_2O , CO_2 , CH_4 , H_2 , CO) at high pressures and temperatures.
2. Proportions of species in the C–O–H system as a function of T at fixed P and f_{O_2} or as a function of f_{O_2} at fixed P and T . Calculations can be made with either ideal or non-ideal mixing using the Van Laar model of Holland & Powell (2003, *CMP* 145, 492–501). The program detects whether to use graphite or diamond in COH calculations depending on the pressure and temperature.
3. Activity-composition relations for binary pairs among H_2O , CO_2 , CH_4 , H_2 , CO species, using the models above.

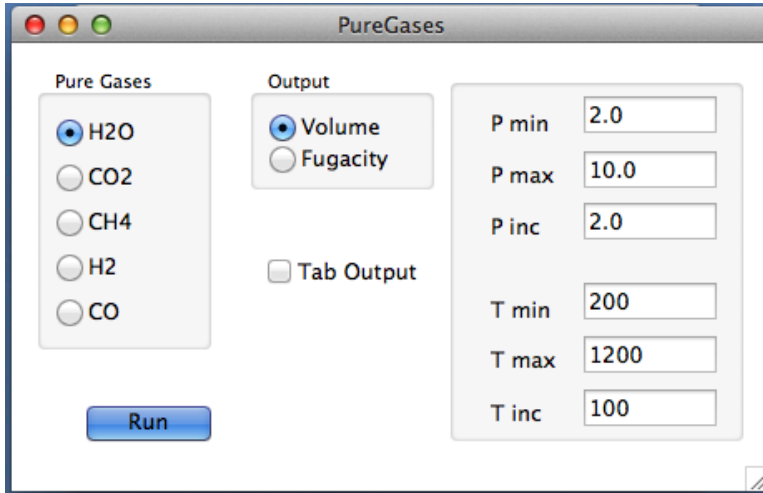
There is an option to use the Pitzer & Sterner equations (1995, *Int J Thermophys* 16, 511–518) in place of the CORK equations, for H_2O and CO_2 only.

Running CHO

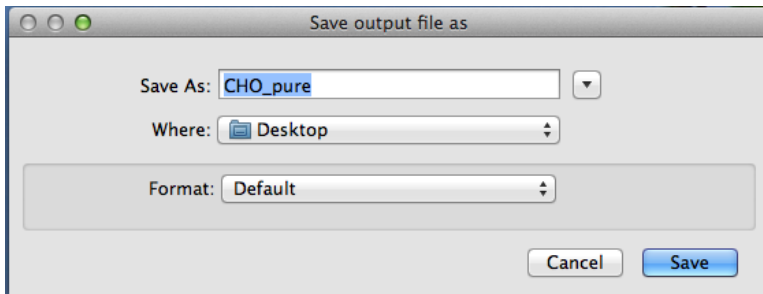
1. **Open** the program and you are presented with the main panel. Here you can set the EOS (Pitzer & Sterner or CORK). The Pitzer & Sterner EOS is used only for H_2O and CO_2 ; for other gases CORK is always used. Then you can choose between the three types of calculation (listed above) by pressing on the appropriate button.



2. **Pure gases:** Pressing the Pure Gases button gives you the gas fugacity and volume panel. Here you can choose the gas, the output mode (volume or fugacity) and set the P and T ranges and increments for tabulating the results. The molar volumes are given in J/bar units and the fugacities are expressed as values for $RT \ln f$ in units of kJ/mol. The tab checkbox allows tab-separated tabular output.



Pressing the Run button prompts you for a file output dialog where you can select the file name and location for your results.



When you press the Save button you will see the results in a window (below) which can be dismissed by pressing the close button on the window bar. You can also open the text file with your favourite text editor.

Uses Pitzer-Sterner EOS												
H2O Volumes J/bar.mol												
T deg C	200.0	300.0	400.0	500.0	600.0	700.0	800.0	900.0	1000.0	1100.0	1200.0	
P kbar	2.000	1.858	2.037	2.271	2.589	3.035	3.607	4.241	4.880	5.499	6.089	6.653
	4.000	1.744	1.870	2.013	2.177	2.370	2.596	2.855	3.139	3.438	3.739	4.038
	6.000	1.667	1.767	1.876	1.994	2.122	2.265	2.423	2.597	2.783	2.977	3.177
	8.000	1.609	1.694	1.784	1.877	1.977	2.083	2.198	2.322	2.455	2.595	2.741
	10.000	1.562	1.636	1.714	1.793	1.875	1.961	2.053	2.150	2.253	2.361	2.475

3. **Mixed Gases:** Pressing the mixed gases option in the main panel brings up the mixed gas panel where you can select the oxygen buffer, the P and the T range and increments for tabulating the results. If you set with graphite, you will get results for gas species H_2O , CO_2 , CH_4 , H_2 , CO in the C–O–H system, otherwise you will get results for H_2O and H_2 in the O–H system. Ideal Mixing may be set in place of Van Laar non-ideal gas mixing. You can refine the $\log f_{O_2}$ value by increasing or decreasing its value relative to the chosen buffer. In the example below the choice is set for 1 log unit below the QFM buffer.

The screenshot shows the 'MixedGases' dialog box with the following settings:

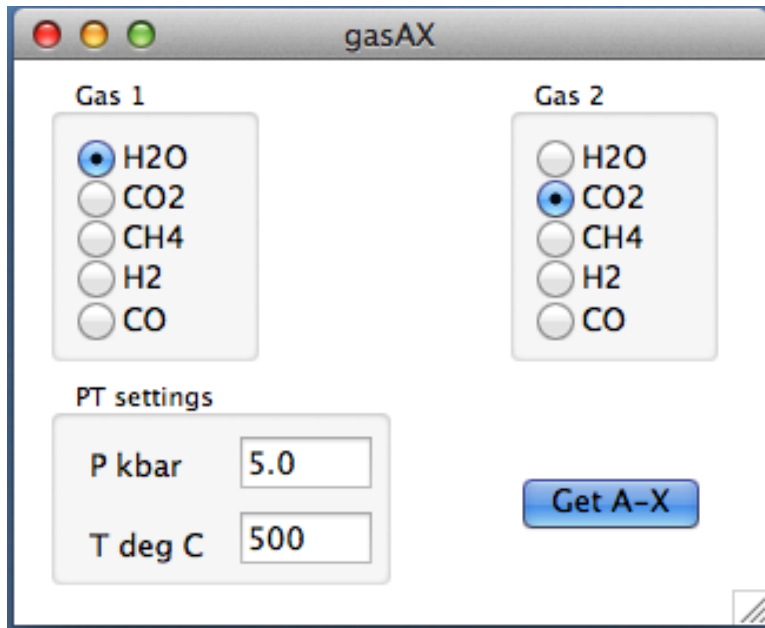
- Oxygen Buffer:** Radio buttons for HM, NNO, QFM (selected), MW, IM, and IW.
- PT settings:** P kbar (5.0), T min (200), T max (1000), T inc (50).
- Log units relative to buffer:** -1
- with graphite/diamond:** checked
- Ideal mixing:** unchecked
- fO2 range (del FMQ):** unchecked
- Run:** button

Ticking the fO2 range box changes the dialog to allow for a range in fo2 expressed as deviations from QFM at specified P and T .

The screenshot shows the 'MixedGases' dialog box with the following settings:

- Oxygen Buffer:** Radio buttons for HM, NNO, QFM, MW, IM, and IW.
- PT settings:** P kbar (5.0), T deg C (1000), fO2 min (-6.0), fO2 max (2.0), fO2 inc (0.5).
- Log units relative to buffer:** -1
- with graphite/diamond:** checked
- Ideal mixing:** unchecked
- fO2 range (del FMQ):** checked
- Run:** button

4. **Gas a-x**: Pressing the Gas a-x button in the main panel brings up the gasAX gas panel where you can select the pair of gases and the P and T for activity-composition calculations. The Van Laar model is used.



In the MixedGas and gasAX options pressing the run or Get A-X button brings up a file dialog for choosing the output file name and location.