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

Introduction

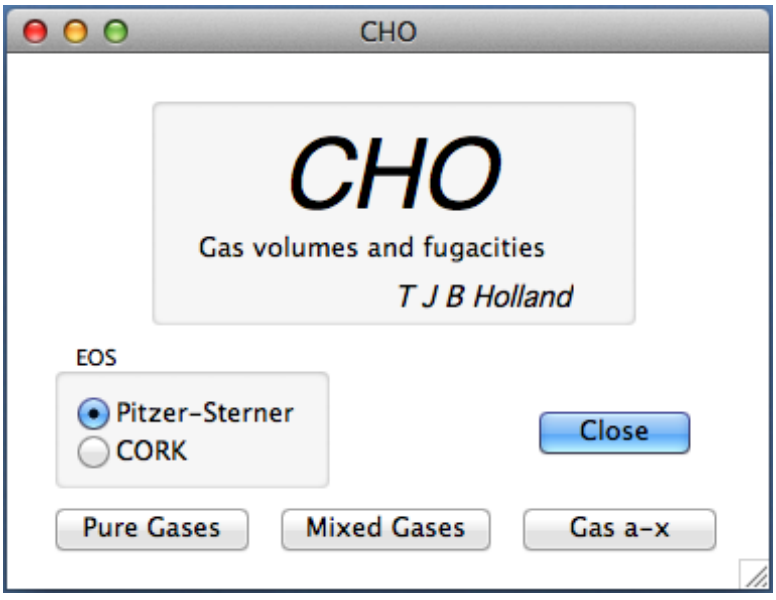
CHO is a program that uses the CORK equation of state (Holland & Powell 1991, *CMP* 109, 265–273) for fluids to calculate the following:

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.

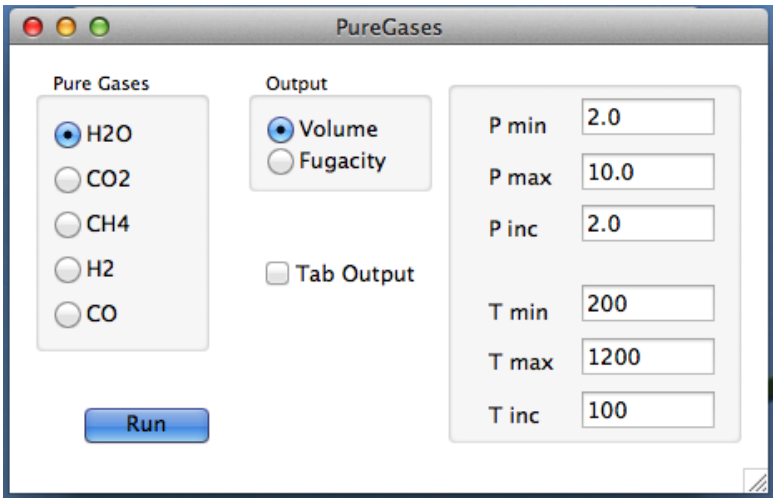
There is an option to use the Pitzer & Sterner equations (1995, *Int J Thermophys* 16, 511–518) in place of the CORK equations, for H_2O and CO_2 only.

Running CHO

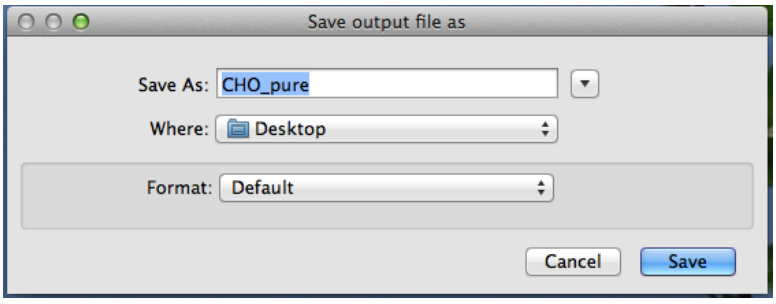
1. **Open** the program and you are presented with the main panel. Here you can set the EOS (Pitzer & Sterner or CORK). The Pitzer & Sterner EOS is used only for H_2O and CO_2; for other gases CORK is always used. Then you can choose between the three types of calculation (listed above) by pressing on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



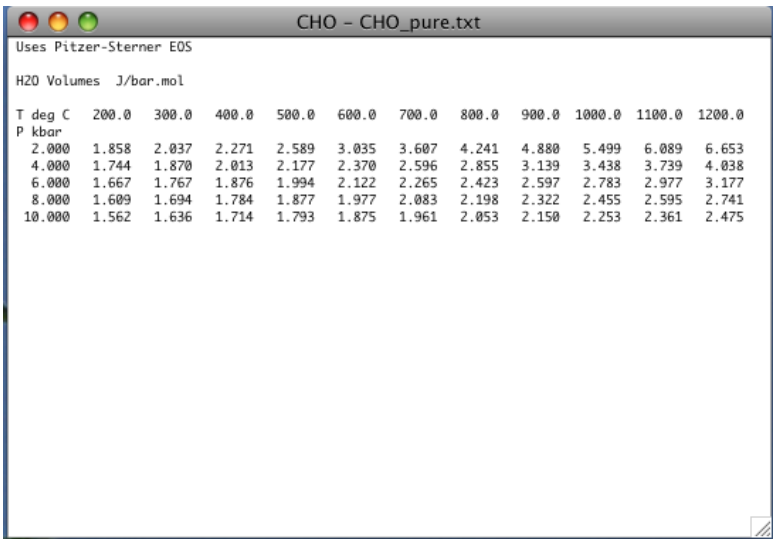
2. **Pure gases**: Pressing the Pure Gases button gives you the gas fugacity and volume panel. Here you can choose the gas, the output mode (volume or fugacity) and set the P and T ranges and increments for tabulating the results. The molar volumes are given in J/bar units and the fugacities are expressed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



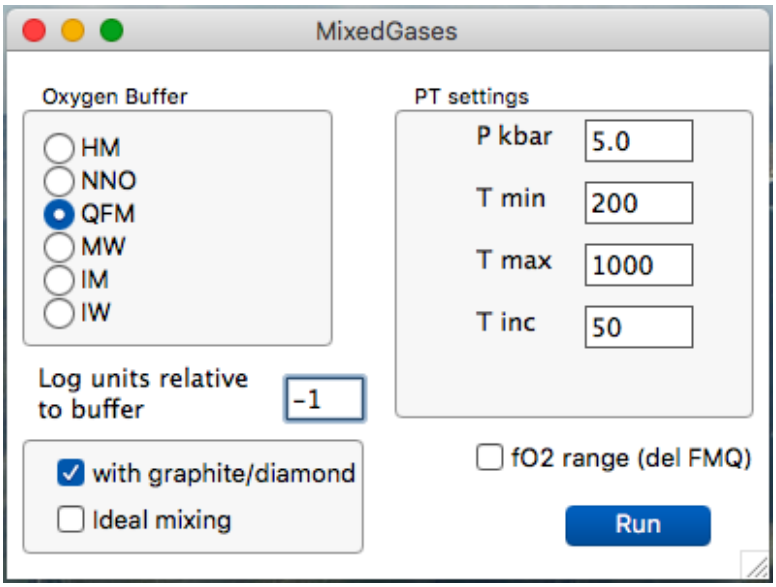
Pressing the Run button prompts you for a file output dialog where you can select the file name and location for your results.



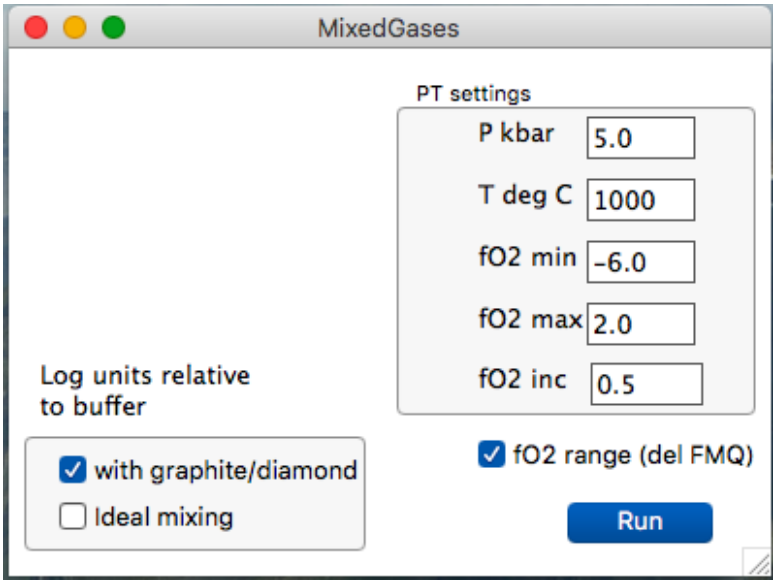
When you press the Save button you will see the results in a window (below) which can be dismissed by pressing the close button on the window bar. You can also open the text file with your favourite text editor.



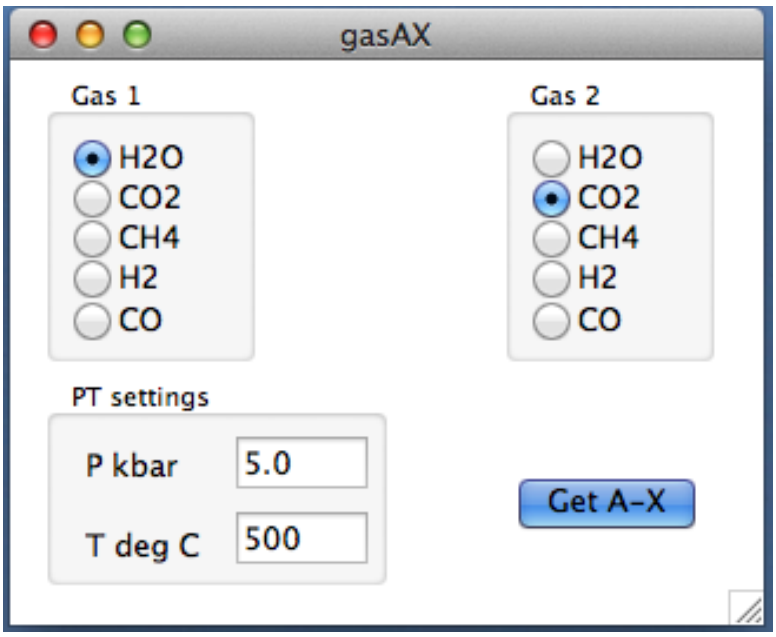
3. **Mixed Gases**: Pressing the mixed gases option in the main panel brings up the mixed gas panel where you can select the oxygen buffer, the P and the T range and increments for tabulating the results. If you set with graphite, you will get results for gas species H_2O, CO_2, CH_4, H_2, CO in the 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.



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.



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.