SOLWCAD

Quick Reference Manual

General information

SOLWCAD computes the fully non-ideal thermodynamic equilibrium between a two-component H_2O+CO_2 fluid and a 12-component (10 major oxides plus dissolved volatiles H_2O and CO_2) silicate melt.

SOLWCAD can be accessed from the web page of Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Pisa: www.pi.ingv.it: within the box "Access to the Volcano Dynamics Computational Centre (VDCC)" click on "Virtual Access", then follow the link to "SOLWCAD". From there, you will access:

1. the user-friendly web-based application (for any user);
2. the stand-alone code provided as an application file (for intermediate level users);
3. the source code provided as a FORTRAN77 routine (for expert users).

This quick manual explains how to use the above three resources. Each of them allows progressively more elaborated calculations, and is treated at different sections inside this manual.

References

Main Reference:

Papale, P., Moretti, R., Barbato, D., The compositional dependence of the saturation surface of H_2O+CO_2 fluids in silicate melts. Chemical Geology 229: 78-95, 2006.

Additional References:

Papale, P., Modeling of the solubility of a two-component H_2O+CO_2 fluid in silicate liquids. American Mineralogist 84: 477-492, 1999.

Papale, P., Modeling of the solubility of a one-component H_2O or CO_2 fluid in silicate liquids. Contributions to Mineralogy and Petrology 126: 237-251, 1997.

Section 1. User-friendly web-based application

1. Select the type of calculation:

   a) Type 1: "P and fluid composition". For any equilibrium pair of dissolved H_2O and CO_2, the entrapment pressure and the composition of the coexisting fluid phase are computed. This is the typical calculation employed in melt inclusion studies.

   b) Type 2: "Fluid-melt volatile partition". For any total amounts of H_2O and CO_2 in the system, the dissolved amounts and the composition of the coexisting fluid phase are computed. This is the classical calculation of the saturation surface.

2. Define H_2O and CO_2. For type 1 calculations, these amounts correspond to the dissolved ones (e.g., the amounts measured in melt inclusions). For type 2 calculations, these amounts correspond to the total amounts in the system, i.e., (mass of each volatile) / (mass of the melt plus mass of the fluid). IMPORTANT NOTE: for both type 1 and type 2 calculations, the defined amounts of H_2O and CO_2 are specified as wt% and are not modified, no matter what is the sum of melt components different from H_2O and CO_2.

3. Define the volatile-free melt composition. This is done by specifying the mass of 10 major oxide components. The units are arbitrary, and the sum does not need to close to any specified value; only the relative amounts matter.

4. Specify pressure (in MPa). This is required for both type 1 and type 2 calculations, but it is used only in type two calculations (as in type 1 calculations, pressure is an output from SOLWCAD).

5. Specify temperature (in °C).

6. Click on "Run". The results will appear nearly immediately.

Section 2. Stand-alone application code

The executable file solwcad runs on Linux systems. Just copy it in a folder and double click (you may need to change its status to executable before being able to launch it. In such a case, open a terminal window; go to the folder containing solwcad; write the following:

chmod 777 solwcad

then press enter. The program can then be executed.

INPUT files

There are two input files: swinput.data and sw.data. Any input quantity is specified in I.S. Units. All quantities are real*8, unless they are specified as integer. An integer quantity must not contain any dot separating decimals, not admitted. A real*8 quantity can be written in different formats. All of the following formats are admitted:
0.34
.34
.3400
.34d0
.0034d2
3.4d-1
3.400d-1
Note that the exponential term must be indicated as "d" (not as "e"). Note also that a dot must appear; e.g., the number 34 in real*8 is written as 34. or 34.d0 or 3.4d1 etc.

The input file **<u>sw.data</u>** includes user-defined conditions in terms of pressure, temperature, and composition, each one arranged on a single row. There is no limitation to the number of rows.

Each row reports the followings:

pressure (Pa)

temperature (K)

H_2O content (wt fraction)**

CO_2 content (wt fraction)**

The following ten quantities specify the volatile-free melt composition (wt fraction)***, in the following order: SiO_2 TiO_2 Al_2O_3 Fe_2O_3 FeO MnO MgO CaO Na_2O K_2O

**H2O and CO2 contents may refer to i) total amounts in the two-phase magma, equal to (mass of volatile in the fluid + mass of volatile dissolved in the melt) / (mass of the gas phase + mass of the melt phase); or ii) the amounts dissolved in the melt phase, that is, (mass of volatile dissolved in the melt) / (mass of the melt phase). The specific choice is determined by the parameter kl in input file swinput.data (see below).

***Volatile-free melt composition can sum up to any number – only relative amounts matter.

The input file **swinput.data** includes specifics for the desired computation. It consists of one line reporting:

`ndat1, ndat2` (integer), refer to the row numbers in sw.data for which computations are desired (see below)

`kl` (integer), it specifies the kind of computation desired:

`kl = 0`	The computation is performed at user-defined P-T conditions in sw.data. H_2O and CO_2 contents in sw.data refer to total amounts in the two-phase magma, or to (mass of volatile component) / (mass of melt + fluid phases). SOLWCAD computes the partitioning of the two volatiles in the fluid and melt phases for user-defined composition. Computations are performed from row `ndat1` to row `ndat2` (only one computation is performed if `ndat1=ndat2`).
`kl = 1`	The computation is performed with reference to row `ndat1` in sw.data, at constant user-defined T and for pressure from user-defined P to atmospheric. At each pressure, a computation similar to the one for kl=0 is performed.
`kl = 2`	Same as for kl=1, but for fixed P (from sw.data) and T from the one in sw.data to a user-defined value `tlimit`, with user-defined T-steps (see below).
`kl = -1`	H_2O and CO_2 in sw.data represent amounts dissolved in the melt phase. For user-defined melt composition and temperature, SOLWCAD returns the equilibrium pressure and composition of the coexisting fluid phase. Computations are performed from row `ndat1` to row `ndat2` (only one computation is performed if `ndat1=ndat2`). This kind of computation is commonly used in the analysis of melt inclusion data.

`iopen` (integer). Put 0 for closed-system calculations, 1 for open system calculations as specified by `fopen` (see below).

`fopen`, only used with `iopen=1`. It specifies the weight fraction of fluid phase lost at each subsequent computation step (when kl=1 or kl=2).

`dt`, the length of the T-steps for use with `kl=2` (either positive or negative).

`tlimit`, the temperature up to which separate computations are performed when `kl=2`. It can be either higher (dt>0) or lower (dt<0) than T.

OUTPUT file

There is only one output file, named **solwcad.out**, consisting of as much rows as the number of single computations performed (as specified in swinput.data).

Each row reports the following quantities in subsequent columns:

Pressure (Mpa)

Temperature (K)

Total (`kl`>0) or dissolved (`kl`=-1) H_2O (wt%)

Total (`kl`>0) or dissolved (`kl`=-1) CO_2 (wt%)

H_2O dissolved in the melt (wt%)

CO_2 dissolved in the melt (ppm)

CO_2 in the fluid (wt%)

CO_2 in the fluid (mol%)

Amount of fluid phase in magma (wt%)

Amount of fluid phase in magma (vol%)

Density of the melt phase** (kg/m^3)

Density of the gas phase (kg/m^3)

Density of the two-phase magma (kg/m^3)

Viscosity of the melt phase*** [log (Pa s)]

Viscosity of the two-phase magma**** [log (Pa s)]

**melt density is computed by the Lange (1994) model
***melt viscosity is computed by the Giordano et al. (2008) model
****the viscosity of bubble-bearing melt is computed by the Ishii and Zuber (1979) model for non-deformable bubbles

Section 3. Source code

The FORTRAN77 source code is provided as a double precision subroutine, named solwcadsub.f, that can be linked to a user-defined code and be called iteratively. There are no common declarations required.

The routine is called with the following command:

```
call solwcad(p,t,ox,xy,igas)
```

All quantities are in SI units.

`p`: pressure (Pa), real*8. It is an input quantity, except when `igas=0` (see below), in which case it is an output quantity.

`t`: temperature (K), real*8. Input.

`ox`: real*8 vector of length 12 reporting (in the order) the contents of: H_2O, CO_2, SiO_2 TiO_2 Al_2O_3 Fe_2O_3 FeO MnO MgO CaO Na_2O K_2O. All terms in the vector are input quantities.

H_2O and CO_2 contents in `ox` must be specified as wt fraction, and can refer to i) total amounts in the two-phase magma, equal to (mass of volatile in the fluid + mass of volatile dissolved in the melt) / (mass of the gas phase + mass of the melt phase); or ii) the amounts dissolved in the melt phase, that is, (mass of volatile dissolved in the melt) / (mass of the melt phase). The specific choice is determined by `igas` (see below).
IMPORTANT NOTE: the amounts of H_2O and CO_2 upon calling SOLWCAD are those at `ox(1)` and `ox(2)`, no matter what is the sum of other oxide components. The sum of all other oxide components `ox(3)-ox(12)`(also in mass fraction) defining the volatile-free melt composition is insubstantial, as only their relative proportions count.

`xy`: real*8 vector of length 4 reporting the amounts of (in the order) dissolved H_2O, dissolved CO_2, H_2O in the fluid phase, CO_2 in the fluid phase, all in wt fraction. For dissolved amounts, the wt fraction corresponds to (mass of dissolved volatile component) / (mass of melt including dissolved volatiles). For the fluid phase, the wt fraction corresponds to (mass of volatile component in the fluid phase) / (mass of the fluid phase) (therefore, `xy(3)+xy(4) = 1`). `xy(1)` and `xy(2)` are output quantities, except when `igas = 0` (see below). `xy(3)` and `xy(4)` are always output quantities.

`igas`: integer with possible values 0,1,2,3, defining the type of calculation desired.

`igas = 0`. This corresponds to type 1 calculations described at section 1 above: given the volatile-free composition specified at `ox(3)-ox(12)`, temperature `t`, and dissolved H_2O and CO_2 contents at `ox(1)` and `ox(2)`, respectively, SOLWCAD returns the equilibrium pressure in `p` and the composition of the coexisting fluid phase in `xy(3)` and `xy(4)`.

`igas = 3`. This corresponds to type 2 calculations described at section 1 above: given the volatile-free composition specified at `ox(3)-ox(12)`, pressure `p`, temperature `t`, and total amounts of H_2O and CO_2 at `ox(1)` and `ox(2)`, respectively, SOLWCAD returns in `xy` the amount of volatiles dissolved in the melt and exsolved in the fluid phase. NOTE: with `igas = 3`, SOLWCAD can be called with either

ox(1) = 0 or ox(2) = 0. In such a case, it will return in xy(1) or xy(2), respectively, the solubility of the corresponding volatile component for pressure below the saturation pressure, and the saturation content corresponding to the specified total amount ox(1) or ox(2), above the saturation pressure.

igas = 1 (or 2). This corresponds to setting igas = 3 and ox(2) = 0 (or ox(1) = 0), no matter what is the specified amount in ox(2) (or ox(1)).

NOTE: after each call of SOLWCAD with igas ≠ 0 the mass fraction of the coexisting gas phase in the system can be computed as (ox(1)+ox(2)-xy(1)-xy(2)) / (1.-xy(1)-xy(2)). For igas = 0 the mass of the coexisting gas phase is not univocally determined (see: Papale, P., Determination of total H2O and CO2 budgets in evolving magmas from melt inclusion data. Journal of Geophysical research 110, d.o.i. 10.1029/2004JB003033, 2005).