

## QUODcarb variable names

QUODcarb's mksys function creates variable names for every parameter in the system. Capitalization does matter, and the capitalization scheme is as follows:

- Default lowercase for all parameter values
  - EXCEPT temperature (T) and pressure (P)
  - EXCEPT a small selection are capitalized to avoid ambiguity
    - HF and F of the fluoride system
      - phf looked too much like free hydrogen ion and 'f' by itself has other uses, so they are HF and F
    - H2S and HS of the sulfide system
      - hs was unclear, in our opinion, so it is HS
    - fH the free hydrogen ion activity coefficient
      - we used fH as in the CO2SYSv3 code
- Default totals all uppercase
  - TC, TA, TB, TS, TF, TP, TSi, TNH4, TH2S, TCa
  - only a trailing letter is lowercase
- Default pK is lowercase p (for -log10), uppercase K, lowercase following letter(s)
  - K0, K1, K2, Kb, Kw, Ks, Kf, Kp1, Kp2, Kp3, Ksi, Knh4, Kh2s, Kar, Kca
  - OmegaCa and OmegaAr fall under this category

## QUODcarb Possible Inputs

\* means it is required

`obs.tp(i).var` can repeat for as many temperature-pressure dependent systems as input

Variable	Name	Units
<code>obs.sal</code>	*salinity	S <sub>p</sub> (unitless)
<code>obs.usal</code>	salinity measurement uncertainty ( $\pm 1$ sigma)	S <sub>p</sub> (unitless)
<code>obs.TC</code>	total carbon, dissolved inorganic carbon (DIC)	$\mu\text{mol/kg-SW}$
<code>obs.uTC</code>	total carbon measurement uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg-SW}$
<code>obs.TA</code>	total alkalinity	$\mu\text{mol/kg-SW}$
<code>obs.uTA</code>	total alkalinity uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg-SW}$
<code>obs.tp(i).T</code>	*temperature	°C
<code>obs.tp(i).uT</code>	temperature uncertainty ( $\pm 1$ sigma)	°C
<code>obs.tp(i).P</code>	*pressure (below surface, surface = 0 dbar)	dbar

obs.tp(i).uP	pressure uncertainty ( $\pm 1$ sigma)	dbar
obs.tp(i).fco2	fugacity of $\text{CO}_2 = f(\text{CO}_2)$	$\mu\text{atm}$
obs.tp(i).ufco2	$f(\text{CO}_2)$ uncertainty ( $\pm 1$ sigma)	$\mu\text{atm}$
obs.tp(i).pco2	partial pressure of $\text{CO}_2 = p(\text{CO}_2)$	$\mu\text{atm}$
obs.tp(i).upco2	$p(\text{CO}_2)$ uncertainty ( $\pm 1$ sigma)	$\mu\text{atm}$
obs.tp(i).co2st	$\text{CO}_2^* = \text{CO}_2(aq) + \text{H}_2\text{CO}_3(aq)$	$\mu\text{atm}$
obs.tp(i).uco2st	$\text{CO}_2^*$ uncertainty ( $\pm 1$ sigma)	$\mu\text{atm}$
obs.tp(i).co3	total carbonate ion = $\text{CO}_3^{2-}\text{T}$	$\mu\text{mol/kg-SW}$
obs.tp(i).uco3	$\text{CO}_3^{2-}\text{T}$ uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg-SW}$
obs.tp(i).ph	$-\log_{10}$ hydrogen ion = pH	unitless
obs.tp(i).uph	pH uncertainty ( $\pm 1$ sigma)	unitless
obs.TB	total borate	$\mu\text{mol/kg-SW}$
obs.uTB	total borate uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg-SW}$
obs.TS	total sulfate	$\mu\text{mol/kg-SW}$
obs.uTS	total sulfate uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg}$
obs.TF	total fluoride	$\mu\text{mol/kg-SW}$
obs.uTF	total fluoride uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg-SW}$
obs.TP	total phosphate = $\text{H}_3\text{PO}_4 + \text{H}_2\text{PO}_4^- + \text{HPO}_4^{2-} + \text{PO}_4^{3-}$	$\mu\text{mol/kg-SW}$
obs.uTP	total phosphate uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg-SW}$
obs.TSi	total silicate	$\mu\text{mol/kg-SW}$
obs.uTSi	total silicate uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg-SW}$
obs.TNH4	total ammonia = $\text{NH}_3 + \text{NH}_4^+$	$\mu\text{mol/kg-SW}$
obs.uTNH4	total ammonia uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg-SW}$
obs.TH2S	total sulfide	$\mu\text{mol/kg-SW}$
obs.uTH2S	total sulfide uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg-SW}$
obs.TCa	total calcium	$\mu\text{mol/kg-SW}$
obs.uTCa	total calcium uncertainty ( $\pm 1$ sigma)	$\mu\text{mol/kg-SW}$

## QUODcarb Possible Outputs

- Every parameter in the system has six possible forms (except a few exceptions):
  - 1 & 2- parameter value and parameter uncertainty in normal space
  - 3 & 4- parameter value and parameter uncertainty in  $-\log_{10}$  space ('p')
  - 5 & 6- upper and lower error bounds in normal space
    - Upper/Lower error bounds are calculated in normal space, they don't exist in  $-\log_{10}$  space ('p')
- `obs.tp(i).var` will repeat for as many temperature-pressure dependent systems as input, `tp(1)`, `tp(2)`, `tp(3)`, etc.
- this list is also available at your command line if you use the command `'fieldnames(est)'` and `'fieldnames(est.tp)'`
  - or `'fieldnames(est(1).tp)'` if more than one datapoint in `est` structure
- Temperature, Salinity, and Pressure
  - `est.sal`, `est.usal`
  - `est.tp(i).T`, `est.tp(i).uT`
  - `est.tp(i).P`, `est.tp(i).uP`
- Total carbon, also known as DIC
  - `est.TC`, `est.uTC`, `est.uTC_u`, `est.uTC_l`
  - `est.pTC`, `est.upTC`
- Total alkalinity
  - `est.TA`, `est.uTA`, `est.uTA_u`, `est.uTA_l`
  - `est.pTA`, `est.upTA`
- Water:  $K_w = [h]/[oh]$ 
  - `Kw`:
    - `est.tp(i).pKw`, `est.tp(i).upKw`, `est.tp(i).Kw`, `est.tp(i).uKw`, `est.tp(i).uKw_u`, `est.tp(i).uKw_l`
  - `oh`:
    - `est.tp(i).poh`, `est.tp(i).upoh`, `est.tp(i).oh`, `est.tp(i).uoh`, `est.tp(i).uoh_u`, `est.tp(i).uoh_l`
  - `ph`:
    - `est.tp(i).ph`, `est.tp(i).uph`, `est.tp(i).h`, `est.tp(1).uh`, `est.tp(i).uh_u`, `est.tp(i).uh_l`
  - `ph` (free scale):
    - `est.tp(i).ph_free`, `est.tp(i).uph_free`, `est.tp(i).h_free`, `est.tp(1).uh_free`, `est.tp(i).uh_free_u`, `est.tp(i).uh_free_l`
  - `ph` (total scale):

- `est.tp(i).ph_tot, est.tp(i).uph_tot,`  
`est.tp(i).h_tot, est.tp(1).uh_tot,`  
`est.tp(i).uh_tot_u, est.tp(i).uh_tot_l`
  - `ph` (seawater scale):
    - `est.tp(i).ph_sws, est.tp(i).uph_sws,`  
`est.tp(i).h_sws, est.tp(1).uh_sws,`  
`est.tp(i).uh_sws_u, est.tp(i).uh_sws_l`
  - `ph` (nbs scale):
    - `est.tp(i).ph_nbs, est.tp(i).uph_nbs,`  
`est.tp(i).h_nbs, est.tp(1).uh_nbs,`  
`est.tp(i).uh_nbs_u, est.tp(i).uh_nbs_l`
- Carbonate:  $K0 = [\text{co2st}]/[\text{fco2}]$ ,  $K1 = [\text{h}][\text{hco3}]/[\text{co2st}]$ ,  $K2 = [\text{h}][\text{co3}]/[\text{hco3}]$ 
  - `K0`:
    - `est.tp(i).pK0, est.tp(i).upK0, est.tp(i).K0,`  
`est.tp(i).uK0, est.tp(i).uK0_u, est.tp(i).uK0_l`
  - `K1`:
    - `est.tp(i).pK1, est.tp(i).upK1, est.tp(i).K1,`  
`est.tp(i).uK1, est.tp(i).uK1_u, est.tp(i).uK1_l`
  - `K2`:
    - `est.tp(i).pK2, est.tp(i).upK2, est.tp(i).K2,`  
`est.tp(i).uK2, est.tp(i).uK2_u, est.tp(i).uK2_l`
  - `fco2`:
    - `est.tp(i).pfco2, est.tp(i).upfco2,`  
`est.tp(i).fco2, est.tp(i).ufco2,`  
`est.tp(i).ufco2_u, est.tp(i).ufco2_l`
  - `co2st`:
    - `est.tp(i).pco2st, est.tp(i).upco2st,`  
`est.tp(i).co2st, est.tp(i).uco2st,`  
`est.tp(i).uco2st_u, est.tp(i).uco2st_l`
  - `p2f`: convert `pco2` to `fco2`
    - `est.tp(i).pp2f, est.tp(i).upp2f, est.tp(i).p2f,`  
`est.tp(i).up2f`
  - `hco3`:
    - `est.tp(i).phco3, est.tp(i).uphco3,`  
`est.tp(i).hco3, est.tp(i).uhco3,`  
`est.tp(i).uhco3_u, est.tp(i).uhco3_l`
  - `co3`:
    - `est.tp(i).pco3, est.tp(i).upco3, est.tp(i).co3,`  
`est.tp(i).uco3, est.tp(i).uco3_u,`  
`est.tp(i).uco3_l`

- Borate:  $K_b = [h][boh4]/[boh3]$ 
  - TB:
    - est.TB, est.uTB, est.uTB\_u, est.uTB\_l, est.pTB, est.upTB
  - Kb:
    - est.tp(i).pKb, est.tp(i).upKb, est.tp(i).Kb, est.tp(i).uKb, est.tp(i).uKb\_u, est.tp(i).uKb\_l
  - boh4:
    - est.tp(i).pboh4, est.tp(i).upboh4, est.tp(i).boh4, est.tp(i).uboh4, est.tp(i).uboh4\_u, est.tp(i).uboh4\_l
  - boh3:
    - est.tp(i).pboh3, est.tp(i).upboh3, est.tp(i).boh3, est.tp(i).uboh3, est.tp(i).uboh3\_u, est.tp(i).uboh3\_l
- Sulfate:  $K_s = [fH][so4]/[hso4]$ 
  - TS:
    - est.TS, est.uTS, est.uTS\_u, est.uTS\_l, est.pTS, est.upTS
  - Ks:
    - est.tp(i).pKs, est.tp(i).upKs, est.tp(i).Ks, est.tp(i).uKs, est.tp(i).uKs\_u, est.tp(i).uKs\_l
  - fH:
    - est.tp(i).pfH, est.tp(i).upfH, est.tp(i).fH, est.tp(i).ufH, est.tp(i).ufH\_u, est.tp(i).ufH\_l
  - so4:
    - est.tp(i).pso4, est.tp(i).upso4, est.tp(i).so4, est.tp(i).uso4, est.tp(i).uso4\_u, est.tp(i).uso4\_l
  - hso4:
    - est.tp(i).phso4, est.tp(i).uphso4, est.tp(i).hso4, est.tp(i).uhso4, est.tp(i).uhso4\_u, est.tp(i).uhso4\_l
- Fluoride:  $K_f = [h][F]/[HF]$ 
  - TF:
    - est.TF, est.uTF, est.uTF\_u, est.uTF\_l, est.pTF, est.upTF
  - Kf:
    - est.tp(i).pKf, est.tp(i).upKf, est.tp(i).Kf, est.tp(i).uKf, est.tp(i).uKf\_u, est.tp(i).uKf\_l

- F:
  - `est.tp(i).pF`, `est.tp(i).upF`, `est.tp(i).F`,  
`est.tp(i).uF`, `est.tp(i).uF_u`, `est.tp(i).uF_l`
- HF:
  - `est.tp(i).pHF`, `est.tp(i).upHF`, `est.tp(i).HF`,  
`est.tp(i).uHF`, `est.tp(i).uHF_u`, `est.tp(i).uHF_l`
- Phosphate:  $Kp1 = [h][h_2po_4]/[h_3po_4]$ ,  $Kp2 = [h][hpo_4]/[h_2po_4]$ ,  $Kp3 = [h][po_4]/[hpo_4]$ 
  - TP:
    - `est.TP`, `est.uTP`, `est.uTP_u`, `est.uTP_l`, `est.pTP`,  
`est.upTP`
  - Kp1:
    - `est.tp(i).pKp1`, `est.tp(i).upKp1`, `est.tp(i).Kp1`,  
`est.tp(i).uKp1`, `est.tp(i).uKp1_u`,  
`est.tp(i).uKp1_l`
  - Kp2:
    - `est.tp(i).pKp2`, `est.tp(i).upKp2`, `est.tp(i).Kp2`,  
`est.tp(i).uKp2`, `est.tp(i).uKp2_u`,  
`est.tp(i).uKp2_l`
  - Kp3:
    - `est.tp(i).pKp3`, `est.tp(i).upKp3`, `est.tp(i).Kp3`,  
`est.tp(i).uKp3`, `est.tp(i).uKp3_u`,  
`est.tp(i).uKp3_l`
  - h3po4:
    - `est.tp(i).ph3po4`, `est.tp(i).uph3po4`,  
`est.tp(i).h3po4`, `est.tp(i).uh3po4`,  
`est.tp(i).uh3po4_u`, `est.tp(i).uh3po4_l`
  - h2po4:
    - `est.tp(i).ph2po4`, `est.tp(i).uph2po4`,  
`est.tp(i).h2po4`, `est.tp(i).uh2po4`,  
`est.tp(i).uh2po4_u`, `est.tp(i).uh2po4_l`
  - hpo4:
    - `est.tp(i).phpo4`, `est.tp(i).uphpo4`,  
`est.tp(i).hpo4`, `est.tp(i).uhpo4`,  
`est.tp(i).uhpo4_u`, `est.tp(i).uhpo4_l`
  - po4:
    - `est.tp(i).ppo4`, `est.tp(i).uppo4`, `est.tp(i).po4`,  
`est.tp(i).upo4`, `est.tp(i).upo4_u`,  
`est.tp(i).upo4_l`
- Silicate:  $Ksi = [h][siooh_3]/[sioh_4]$

- TSi:
  - est.TSi, est.uTSi, est.uTSi\_u, est.uTSi\_l, est.pTSi, est.upTSi
- Ksi:
  - est.tp(i).pKsi, est.tp(i).upKsi, est.tp(i).Ksi, est.tp(i).uKsi, est.tp(i).uKsi\_u, est.tp(i).uKsi\_l
- siooh3:
  - est.tp(i).psiooh3, est.tp(i).upsiooh3, est.tp(i).siooh3, est.tp(i).usiooh3, est.tp(i).usiooh3\_u, est.tp(i).usiooh3\_l
- sioh4:
  - est.tp(i).psioh4, est.tp(i).upsioh4, est.tp(i).sioh4, est.tp(i).usioh4, est.tp(i).usioh4\_u, est.tp(i).usioh4\_l
- Ammonia:  $\text{Knh4} = [\text{h}][\text{nh3}]/[\text{nh4}]$ 
  - TNH4:
    - est.TNH4, est.uTNH4, est.uTNH4\_u, est.uTNH4\_l, est.pTNH4, est.upTNH4
  - Knh4:
    - est.tp(i).pKnh4, est.tp(i).upKnh4, est.tp(i).Knh4, est.tp(i).uKnh4, est.tp(i).uKnh4\_u, est.tp(i).uKnh4\_l
  - nh3:
    - est.tp(i).pnh3, est.tp(i).upnh3, est.tp(i).nh3, est.tp(i).unh3, est.tp(i).unh3\_u, est.tp(i).unh3\_l
  - nh4:
    - est.tp(i).pnh4, est.tp(i).upnh4, est.tp(i).nh4, est.tp(i).unh4, est.tp(i).unh4\_u, est.tp(i).unh4\_l
- Sulfide:  $\text{Kh2s} = [\text{h}][\text{HS}]/[\text{H2S}]$ 
  - TH2S:
    - est.TH2S, est.uTH2S, est.uTH2S\_u, est.uTH2S\_l, est.pTH2S, est.upTH2S
  - Kh2s:
    - est.tp(i).pKh2s, est.tp(i).upKh2s, est.tp(i).Kh2s, est.tp(i).uKh2s, est.tp(i).uKh2s\_u, est.tp(i).uKh2s\_l
  - HS:

- est.tp(i).pHS, est.tp(i).upHS, est.tp(i).HS, est.tp(i).uHS, est.tp(i).uHS\_u, est.tp(i).uHS\_l
- H2S:
  - est.tp(i).pH2S, est.tp(i).upH2S, est.tp(i).H2S, est.tp(i).uH2S, est.tp(i).uH2S\_u, est.tp(i).uH2S\_l
- Aragonite:  $Kar = [co3][ca]/\Omega_{Ar}$ 
  - TCa:
    - est.TCa, est.uTCa, est.uTCa\_u, est.uTCa\_l, est.pTCa, est.upTCa
  - Kar:
    - est.tp(i).pKar, est.tp(i).upKar, est.tp(i).Kar, est.tp(i).uKar, est.tp(i).uKar\_u, est.tp(i).uKar\_l
  - ca:
    - est.tp(i).pca, est.tp(i).upca, est.tp(i).ca, est.tp(i).uca, est.tp(i).uca\_u, est.tp(i).uca\_l
  - $\Omega_{Ar}$ :
    - est.tp(i).p $\Omega_{Ar}$ , est.tp(i).up $\Omega_{Ar}$ , est.tp(i). $\Omega_{Ar}$ , est.tp(i).u $\Omega_{Ar}$ , est.tp(i).u $\Omega_{Ar}$ \_u, est.tp(i).u $\Omega_{Ar}$ \_l
- Calcite:  $Kca = [co3][ca]/\Omega_{Ca}$ 
  - Kca:
    - est.tp(i).pKca, est.tp(i).upKca, est.tp(i).Kca, est.tp(i).uKca, est.tp(i).uKca\_u, est.tp(i).uKca\_l
  - $\Omega_{Ca}$ :
    - est.tp(i).p $\Omega_{Ca}$ , est.tp(i).up $\Omega_{Ca}$ , est.tp(i). $\Omega_{Ca}$ , est.tp(i).u $\Omega_{Ca}$ , est.tp(i).u $\Omega_{Ca}$ \_u, est.tp(i).u $\Omega_{Ca}$ \_l
- Organic Alkalinity:  $Kalpha = [h][alpha]/[halpha]$ 
  - If opt.pKalpha = 1
  - TAlpha:
    - est.TAlpha, est.uTAlpha, est.uTAlpha\_u, est.uTAlpha\_l, est.pTAlpha, est.upTAlpha
  - Kalpha:
    - est.tp(i).pKalpha, est.tp(i).upKalpha, est.tp(i).Kalpha, est.tp(i).uKalpha, est.tp(i).uKalpha\_u, est.tp(i).uKalpha\_l
  - alpha:



- est.tp(i).palpha, est.tp(i).upalpha, est.tp(i).alpha, est.tp(i).ualpha, est.tp(i).ualpha\_u, est.tp(i).ualpha\_l
  - halpha:
    - est.tp(i).phalpha, est.tp(i).uphalpha, est.tp(i).halpha, est.tp(i).uhalpha, est.tp(i).uhalpha\_u, est.tp(i).uhalpha\_l
- Organic Alkalinity:  $K_{\text{beta}} = \frac{[h][\text{beta}]}{[h\text{beta}]}$ 
  - If opt.pKbeta = 1
  - TBeta:
    - est.TBeta, est.uTBeta, est.uTBeta\_u, est.uTBeta\_l, est.pTBeta, est.upTBeta
  - Kbeta:
    - est.tp(i).pKbeta, est.tp(i).upKbeta, est.tp(i).Kbeta, est.tp(i).uKbeta, est.tp(i).uKbeta\_u, est.tp(i).uKbeta\_l
  - beta:
    - est.tp(i).pbeta, est.tp(i).upbeta, est.tp(i).beta, est.tp(i).ubeta, est.tp(i).ubeta\_u, est.tp(i).ubeta\_l
  - hbeta:
    - est.tp(i).phbeta, est.tp(i).uphbeta, est.tp(i).hbeta, est.tp(i).uhbeta, est.tp(i).uhbeta\_u, est.tp(i).uhbeta\_l
- est.f
  - residual 'f' value for internal consistency analysis