

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

obs.tp(i).uP	pressure uncertainty (± 1 sigma)	dbar
obs.tp(i).fco2	fugacity of $\text{CO}_2 = f(\text{CO}_2)$	μatm
obs.tp(i).ufco2	$f(\text{CO}_2)$ uncertainty (± 1 sigma)	μatm
obs.tp(i).pco2	partial pressure of $\text{CO}_2 = p(\text{CO}_2)$	μatm
obs.tp(i).upco2	$p(\text{CO}_2)$ uncertainty (± 1 sigma)	μatm
obs.tp(i).co2st	$\text{CO}_2^* = \text{CO}_2(aq) + \text{H}_2\text{CO}_3(aq)$	μatm
obs.tp(i).uco2st	CO_2^* uncertainty (± 1 sigma)	μatm
obs.tp(i).co3	total carbonate ion = CO_3^{2-}T	$\mu\text{mol/kg-SW}$
obs.tp(i).uco3	CO_3^{2-}T uncertainty (± 1 sigma)	$\mu\text{mol/kg-SW}$
obs.tp(i).ph	$-\log_{10}$ hydrogen ion = pH	unitless
obs.tp(i).uph	pH uncertainty (± 1 sigma)	unitless
obs.TB	total borate	$\mu\text{mol/kg-SW}$
obs.uTB	total borate uncertainty (± 1 sigma)	$\mu\text{mol/kg-SW}$
obs.TS	total sulfate	$\mu\text{mol/kg-SW}$
obs.uTS	total sulfate uncertainty (± 1 sigma)	$\mu\text{mol/kg}$
obs.TF	total fluoride	$\mu\text{mol/kg-SW}$
obs.uTF	total fluoride uncertainty (± 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 (± 1 sigma)	$\mu\text{mol/kg-SW}$
obs.TSi	total silicate	$\mu\text{mol/kg-SW}$
obs.uTSi	total silicate uncertainty (± 1 sigma)	$\mu\text{mol/kg-SW}$
obs.TNH3	total ammonia = $\text{NH}_3 + \text{NH}_4^+$	$\mu\text{mol/kg-SW}$
obs.uTNH3	total ammonia uncertainty (± 1 sigma)	$\mu\text{mol/kg-SW}$
obs.TH2S	total sulfide	$\mu\text{mol/kg-SW}$
obs.uTH2S	total sulfide uncertainty (± 1 sigma)	$\mu\text{mol/kg-SW}$
obs.TCa	total calcium	$\mu\text{mol/kg-SW}$
obs.uTCa	total calcium uncertainty (± 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`
 - Ω_{Ar} :
 - `est.tp(i).p0megaAr, est.tp(i).up0megaAr,`
`est.tp(i).0megaAr, est.tp(i).u0megaAr,`
`est.tp(i).u0megaAr_u, est.tp(i).u0megaAr_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`
 - Ω_{Ca} :
 - `est.tp(i).p0megaCa, est.tp(i).up0megaCa,`
`est.tp(i).0megaCa, est.tp(i).u0megaCa,`
`est.tp(i).u0megaCa_u, est.tp(i).u0megaCa_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: $K_{\text{beta}} = \frac{[\text{h}][\text{beta}]}{[\text{hbeta}]}$
 - If $\text{opt.p}K_{\text{beta}} = 1$
 - `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