AugerQuant appendix (mostly explanation of data structures)

Important parameters in AESquantparams
Negpeak – ideal energy for negative peak in smooth-differentiated spectrum (S7D7)
Pospeak – ideal energy for associated positive peak in S7D7 (lower energy than negpeak
Peakwidth –ideal smooth-diff peak width (which is negpeak-pospeak) in eV
Searchwidth – allowable energy shift for negpeak for given element (in eV).. default is 10eV
which should be fine unless sample is charging significantly
kfactor – this is element's k-factor for smooth-differentiated quant method (determined from
standards)
Mass- atomic mass of this element
Integpeak: energy of direct counts peak (relative to that of negpeak S7D7)… i.e. if S smoothdiff
peak is found at 154eV then algorithms search for direct peak at 3.7 eV lower (near 150.3eV)..
this direct peak is typically found at 4-6eV lower energy than negpeak position
Lower1, lower2, upper1,upper2 are again energies defined relative to negpeak that help find
linear regions away from peak to use for background fits
> **Lower1 and Lower2:** energy range of lower energy linear background fit (relative to ideal
> negpeak position
> **Upper1 and Upper 2:** energy range of upper energy linear background fit (relative to ideal
> negpeak position
Kfactor2—k-factor for given element for direct integral quantification method
windowshift: size adjustment of background region for fitting above and below peaks of interest
in # of channels (where 1channel=1eV typically); used by integquant scripts; shift in fitted region
only occurs if this expanded region doesn't show evidence of a peak or peak edge
Fittype: type of fit to apply to background. Currently cubic and linear are used along with Ca
(which gets special treatment due to large interference from adjacent C peak); it is fairly
straightforward to write new functions to handle different types of peaks and then use this flag to
decide which of the background fitting functions to call;
Integwidth =# of channels for integration of direct counts (full width so includes center channel
plus n/2-1 channels on either side; set to 9 channels for all peaks except Si2 at 13 based on
Gaussian fits of subtracted peaks … using 1.2* FHWM (and FWHM is in turn 2.35*width
returned by Gaussian function)
Siglevel – Ratio of above which direct peak is clearly real; this threshold can zero out a given
composition from integcomp
Comments - element-specific notes about the parameters

Output from smdifquant
Smdifpeakslog contains:
Obvious stuff: **project, filepath, date, sample, filename, filenumber**

Peakenergy , **Peakindex**– actual found value of negative peak in smooth-diff spectrum at peak's high energy edge (in eV and index #s respectively), allowed to shift by n channels depending on peak's searchwidth setting in AESquantparams

PeakID – name of peak (not element name since often multiple peaks per element), defined in AESquantparams

Shift- shift of peak from ideal position listed in AESquantparams.. in index # and assumes 1eV per channel (so # of indices=# of eV)… probably should generalize this sometime to allow for different energy resolutions

Negintensity: Y value at x val defined by peakenergy/peakindex

Posintensity: Y value at high point on low energy side of smdiff peak, algorithm looks n channels to the left (depending on peakwidth setting in AESquantparams, but also allowed to shift from that position by n (based on searchwidth)

Pospeak: energy value where the positive peak is found

Amplitude: peak-to-peak value (posintensity- negintensity)

Peakwidth: peakenergy (defined as negative peak at right edge) – pospeak

Lowback, lowbackamplitude, highback, highbackamplitude, avgbackamplitude – not very reliable measure of background noise (see backreg description below)

Quantdetails: quant run date and params from this peak

Comments: optional field

Adjamp: added later by calcadjamp function, basically it's amplitude*kfactor/mass to allow conversion of these amplitudes into actual compositions … see Stadermann et al. (2009) GCA

Output from integquant

Integquantlog.csv contains:

Filenumber, Filename, Filepath, Sample, Comment, Area-- standard stuff copied from AugerParamLog (area is areanumber of given spatial area)

Element - obvious

Integcounts: peak minus background fit integrated over integwidth (which is roughly ~1.2* FWHM of peak

Backcounts - # of counts under background fit (same integration width and range)

Significance- integcounts/sqrt(background counts)… so value of 2 means actual peak counts are 2 sigma that of the background

Xc, Width, Peakarea, Y0, Rsquared – parameters from Gaussian fit over subtracted peak data (subtracted data is raw counts minus the background fit

Numchannels: number of channels for integration to get integcounts under peak; normally value is 9 channels (although currently it outputs half width 2*numchannels+1 = FWHM) so 4 channels implies integration of center channel plus 4 on either side

Adjcnts: adjusted counts is integcounts * kfactor2/mass – *this is k-factor modified counts and is the quantity from which atomic percents are directly calculated; kfactor2 is for integral method from AESquantparams whereas kfactor is for smooth-diff method*

Erradjcnts: Raw error in adjcnts (adjusted counts as defined above) value**,** including 2 sigma errors from counting statistics and error in the determined k-factor

Backfitlog contents:
Contains details of all the background fits for all spe files, all areas, all chosen peaks
Log file with various common params: filenumber, filename, filepath, sample, comments, date area, element
Lower1, lower2, upper1,upper2: index #s of data in the energy range included in fit (lower1&2 are boundaries of region below peak and upper1 &2 are above peak; default positions in index # (eV) for fits above and below, these regions are adjusted based on shift of deriv peak; modfitregions function also makes fine adjustments to chosen background fit regions

Lowrange, highrange: same as above but in eV (not index #s)
Peakshift: # of eV (same as index #s) that integration window was shifted for this element (allowable shift for each element can be limited using peakshift column in AESquantparams
Fittype: type of background fit as entered in AESquantparams (each type of background handled with different function
P1, P2, P3, P4: fit parameters returned from cubic, linear, and other fit types (i.e. for cubic P1-P4 are A, B, C, D where
Rval1—coeff of determination calculated for this fit (manual calc on curve_fit cubic and automatically returned by linregress for linear fits
Pval1, Stderr1 – P value and standard error returned by linregress (not determined for curve_fit cubic and other fits
Rval2, Pval2, Stderr2 – only defined for interpolated linear fits (not commonly used)