Raddose-3D InputFile Help

All entries are in the format **keyword (argument1 type) (argument3 type)..** Keywords must be reproduced exactly. Entries with a \* are compulsory.

**\*CrystalDim (double1) (double2) (double3):** double1: the size of the crystal in um orthogonal to both the beam and the goniometer at L=P=0. double2: the size of the crystal in um along the goniometer axis at L=P=0. double3: the size of the crystal in um along the beam axis.

**CrystalPixPerUM (double):** the resolution of the grid used to calculate dose in voxels/um. Defaults to 0.5

**Tag (string) :** the tag for the filename of output files. Files will be in formate string-filetype.x e.g string-info.txt. This defaults to the input file name.

**CrystP (double):** the ‘in Plane of loop’ angle between the ydim axis and the goniometer axis. Defaults to 0.

**CrystL (double):** the Loop angle between the plane of the loop and the goniometer axis. Defaults to 0.

**HistRange (double1) (double2):** double1: the minimum dose bin in histograms. double2: the maximum dose bin in histograms. Defaults to 10 40

**HistNBins (integer):** the number of dose bins to be used in histograms. Defaults to 5

**FineHistRange**: Same as HistRange, but for the fine histogram (the one used for energy surface thresholds & the output histogram csv.) Defaults to 0.01 100

**FineHistNBins**: Same as HistNBins, but for the finehist. Defaults to 1001

**AbsEnDoseThreshold**: the fraction of the absorbed energy that is enclosed for the calculation of volume used in average dose. Default 0.95

**DDMType (string):** At this stage, the string must be ‘Simple’. Defaults to simple (yes, this does nothing atm).

**\*CoefCalcType (string1) *(string2)*:** IF string1 is ‘**Dummy’**, no string2. IF string1 is ‘**RDV2FromFile’**, string2 must be the full name of a file containing a correctly formated RADDOSE-V2 input file. String1 must be one of these two options.

**NumWedges (integer)** If multiple wedges are to be used, this parameter must be specified, where the integer is >= 2. Each of the following parameters must then have an extra integer inserted between the parameter name and the arguments with the wedge number (1 for the 1st wedge, 2 for the 2nd etc.)

**\*BeamType (string):** must be either ‘**Gaussian’** or ‘**TopHat’**. IF it is Gaussian, you must specify FWHM for the beam.

**WedgeAngRes (double):** the step size used for wedge iterations. Defaults to 2 degrees.

**WedgeStartAng (double):** Start angle of the rotation, assuming the front face of the crystal (double1-double2 plane) is normal to the beam. Rotation is right handed from????????. Defaults to 0.

**WedgeEndAng (double):** End angle of the rotation. Defaults to 0.

**\*WedgeTotSec (double):** total exposure time in seconds.

**WedgeStart (double1) (double2):** start position of the wedge. offset of the centre of rotation of the crystal from its middle in (normal to beam-goniometer) (goniometer axis). Default (0,0)

**RotAxBeamOffset (double):** the vertical offset between the goniometer and beam axis. Used for precession.

**WedgeTrans (double1) (double2):** translation of the goniometer during exposure in um/degree. double1: of the goniometer-axis/beam-axis offset. double2: along goniometer axis. Defaults to 0, 0.

**\*BeamSize (double1) (double2):** the size of the beam (vertical), (horizontal). This is defined by the slits. For an uncolimated Gaussian beam, set to ~3xFWHM.

**\*BeamFWHM (double1) (double2): ):** the FWHM of the beam (vertical), (horizontal). Not needed if TopHat beam used.

**\*BeamFlux (double):** Total beam flux in photons/sec. scientific (e.g 1e12) notation is acceptable.

**\*BeamEnergy (double):** Energy of the beam in KeV