

RADDOSE-3D GUI

TRY our new GUI written by Josh Dickerson (jdickerson@berkeley.edu)!!

To run RADDOSE-3D for MX, SMX, SAXS (whichever you like!), RADDOSE-XFEL (+ Monte-Carlo simulations) or RADDOSE-ED

Step 1: Download and unzip the RADDOSE-3D GUI from:

[GitHub - GarmanGroup/RADDOSE-3D](#)

There are versions for a PC (Windows_release.zip) and for Linux (Linux_release.zip).

If you have a MAC, there is no new GUI yet, but you can run a limited capability RADDOSE-3D from the WWW site:

raddo.se (click on ‘manual interface’ and run the test example first. Then edit the input for a case you would like to try)

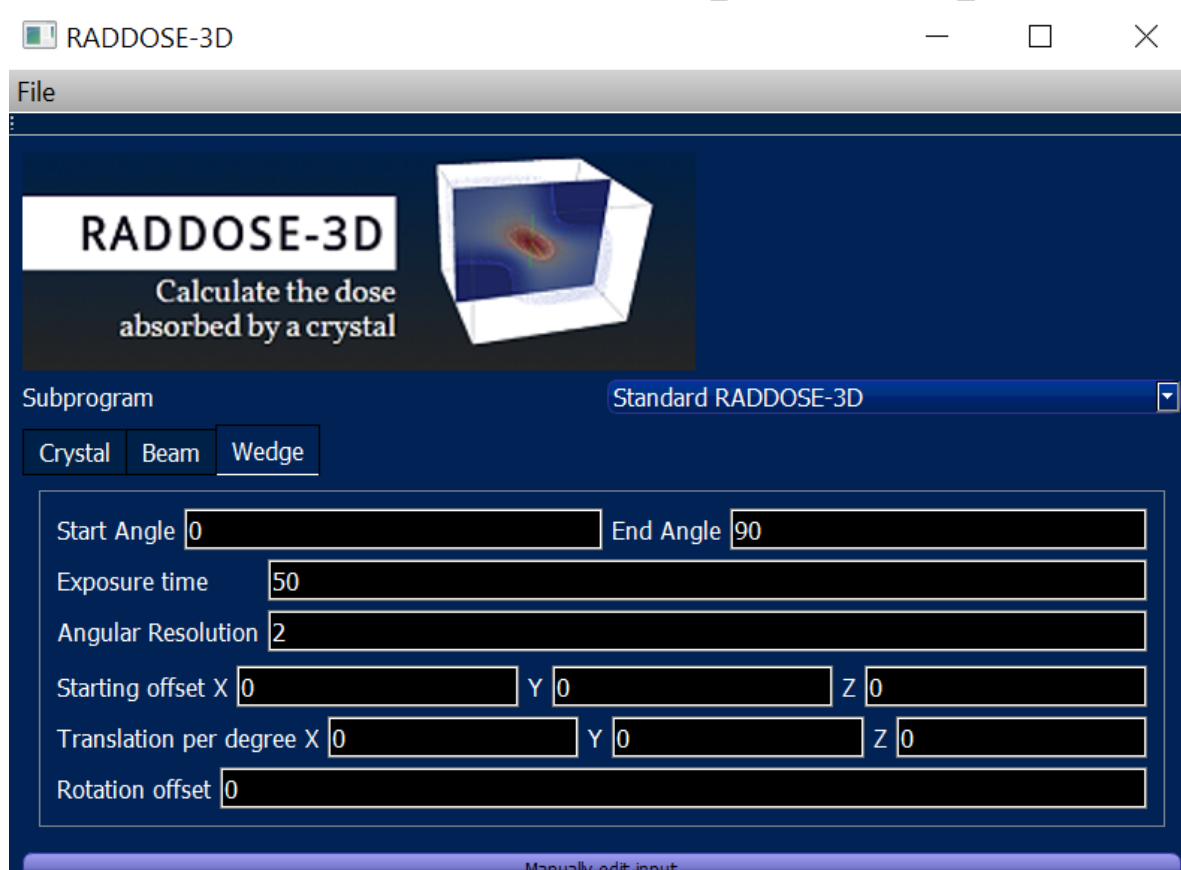
To run the GUI you need to have Java installed which you can get free at

https://www.java.com/download/ie_manual.jsp

Also, if you have R (<https://www.r-project.org/>) installed, from the RADDOSE-3D output you will be able to produce 3D representations of the dose distribution in your sample.

- **Step 2:** Unzip the file you have downloaded. On Windows machines Josh recommends the best place to install the executable (e.g. Documents versus Program Files) is in Documents as he tends to avoid putting programs in Program Files unless he is using an installer, to avoid the need for admin privileges and to keep things self-contained.
- Note that installing a third party executable by direct download rather than through an installer might lead your antivirus software to complain.

Step 3: Find the file RD3D_GUI.EXE and if on a PC click on it. For Linux run it however you usually run executable files. The GUI should open, and you can enter input on 3 tabs: crystal, beam and wedge. See the RADDOSE-3D Manual (link on raddo.se) if you are not familiar with the required input.



Wedge 1:

Collecting data for a total of 50.0s from $\phi = 0.0$ to 90.0 deg.

Crystal coefficients calculated with RADDOSE-3D.

Photoelectric Coefficient: $3.21\text{e-}04$ / μm .

Inelastic Coefficient: $1.86\text{e-}05$ / μm .

Elastic Coefficient: $2.10\text{e-}05$ / μm .

Attenuation Coefficient: $3.61\text{e-}04$ / μm .

Density: 1.14 g/ml.

Average Diffraction Weighted Dose : 6.238509 MGy

Last Diffraction Weighted Dose : 10.508146 MGy

Elastic Yield : $2.27\text{e+}11$ photons

Diffraction Efficiency (Elastic Yield/DWD): $3.64\text{e+}10$ photons/MGy

Average Dose (Whole Crystal) : 5.921152 MGy

Average Dose (Exposed Region) : 5.921152 MGy

Max Dose : 37.291488 MGy

Average Dose (95.0 % of total absorbed energy threshold (2.85 MGy)): 9.501849 MGy

Dose Contrast (Max/Threshold Av.) : 3.92

Used Volume : 100.0%

Absorbed Energy (this Wedge) : $6.88\text{e-}03$ J.

Dose Inefficiency (Max Dose/mJ Absorbed) : 5.4 1/g

Dose Inefficiency PE (Max Dose/mJ Deposited): 5.5 1/g

Final Dose Histogram:

Bin 1, 0.0 to 0.1 MGy: 16.6 %

Bin 2, 0.1 to 3.4 MGy: 26.1 %

Bin 3, 3.4 to 6.7 MGy: 21.0 %

Bin 4, 6.7 to 10.1 MGy: 16.0 %

Bin 5, 10.1 to 13.4 MGy: 9.4 %

Bin 6, 13.4 to 16.7 MGy: 5.0 %

Bin 7, 16.7 to 20.0 MGy: 1.8 %

Bin 8, 20.0 to 23.4 MGy: 1.6 %

Bin 9, 23.4 to 26.7 MGy: 1.0 %

Bin 10, 26.7 to 30.0 MGy: 1.2 %

Bin 11, 30.0 MGy upwards: 0.3 %

RADDOSE-3D terminated after 0.9 seconds

Plot dose histogram

Back

**Step 4: Understanding the output! DOSE = ENERGY
ABSORBED/MASS**

Photoelectric Coefficient: $6.35\text{e-}04$ /um.

Inelastic Coefficient: $1.87\text{e-}05$ /um.

Elastic Coefficient: $2.36\text{e-}05$ /um.

Attenuation Coefficient: $6.77\text{e-}04$ /um.

Density: 1.16 g/ml.

Average Diffraction Weighted Dose : 11.887135 MGy

Last Diffraction Weighted Dose : 20.040846 MGy

Elastic Yield : $2.51\text{e+}11$ photons

Diffraction Efficiency (Elastic Yield/DWD): $2.11\text{e+}10$ photons/MGy

Average Dose (Whole Crystal) : 11.271797 MGy

Average Dose (Exposed Region) : 11.271797 MGy

Max Dose : 71.040785 MGy

Step 4: Understanding the output! DOSE = ENERGY
ABSORBED/MASS

Average Dose (95.0 % of total absorbed energy threshold (5.36
MGy)): 18.088188 MGy

Dose Contrast (Max/Threshold Av.) : 3.93

Used Volume : 100.0%

Absorbed Energy (this Wedge) : 1.33e-02 J.

Dose Inefficiency (Max Dose/mJ Absorbed) : 5.3 1/g

Dose Inefficiency PE (Max Dose/mJ Deposited): 5.5 1/g

NB: some dose is escaping with photoelectrons emerging from
crystal so Max dose/energy absorbed is less than Max dose/energy
deposited)

RADDOSE-3D References

- 1) RADDOSE-3D: time- and space-resolved modeling of dose in macromolecular crystallography. Oliver B. Zeldin, Markus Gerstel and Elspeth F. Garman. *Journal of Applied Crystallography* (2013) 46, 1225-1230.
- 2) Predicting the X-ray lifetime of protein crystals. Oliver B. Zeldin, Sandor Brockhauser, John Bremridge, James Holton and Elspeth F. Garman. *PNAS* (2013) 110, 20551-20556
- 3) Development of tools to automate quantitative analysis of radiation damage in SAXS experiments. Jonathan C. Brooks-Bartlett, Rebecca A. Batters, Charles S. Bury, Edward D. Lowe, Helen Mary Ginn, Adam Round and Elspeth F. Garman. *J. Synchrotron Radiation* (2017) 24, 63–72. doi:10.1107/S1600577516015083
- 4) Estimate your dose: RADDOSE-3D. Charles S. Bury, Jonathan C. Brooks-Bartlett, Steven P. Walsh & Elspeth F. Garman. *Protein Science* (2018) 27, 217–228
- 5) Radiation damage in small molecule crystallography: fact not fiction. Jeppe Christensen, Peter N. Horton, Charles S. Bury, Joshua L. Dickerson, Helena Taberman, Elspeth F. Garman*, Simon J. Coles*. *IUCrJ* (2019) 6, 703–713
- 6) Doses for experiments with microbeams and microcrystals :Monte Carlo simulations in RADDOSE-3D. Joshua L. Dickerson and Elspeth F. Garman. *Protein Science* (2021) 30, 8–19.
- 7) RADDOSE-XFEL: Femtosecond time-resolved dose estimates for macromolecular XFEL experiments. Joshua L. Dickerson, Patrick T.N. McCubbin and Elspeth F. Garman. *J. Appl. Cryst.* (2020). 53, 549–560 <https://doi.org/10.1107/S1600576720000643>
- 8) Recent developments in RADDOSE-3D. Joshua L. Dickerson, Patrick T.N. McCubbin and Elspeth F. Garman (2024) *Protein Science*).