Descriptions of Manhattan Project Physics Spreadsheets
Last update: 21 November 2010

In general, values in these spreadsheets that are intended for user-adjustment appear in **bold red** type. Physical constants and conversion factors appear in **bold blue** and computed values in plain black type. Brief descriptions of each spreadsheet appear below:

BarrierCubic   Calculates and displays the fission barrier function (Fig. 1.11) and linear and cubic models of fission energetics f_{linear} and f_{smooth} (Fig. 1.10) of the "two-sphere" model of fission discussed in Section 1.10. The user specifies only the mass ratio of the fission products and the Coulomb and surface-energy parameters a_C and a_S; the graphs are automatically updated. In a separate block, the user can specify the atomic and nucleon numbers Z and A for some specific case; the barrier energy for that case is computed, taking into account the "offset" value predicted for the model for $(Z, A) = (1,1)$.

Boron   Calculates the maximum tolerable number fraction of Boron atoms in a graphite-moderated reactor and the probability that a neutron scattering within the graphite + Boron mixture will survive N scatters. There are two user-adjustable parameters: (i) the maximum tolerable neutron-capture cross-section, and, (ii) the value of N. The maximum tolerable Boron number fraction is computed and expressed both directly and in "1 part in …" format.

CriticalityAnalytic   For calculating the critical mass of a fission core in two cases: (i) untamped threshold criticality, and (ii) tamped threshold criticality. Also computes (iii) the efficiency and yield for an untamped core of specified mass which exceeds the mass computed in (i). [For the efficiency and yield of a tamped core that exceeds the mass computed in (ii), see CriticalityNumerical.] For (i), the user enters the density, atomic weight, fission cross-section, elastic-scattering cross-section and secondary neutron number of core material. Within a block of cells labeled *Untamped Threshold ("bare") Criticality*, the user then employs the Goal Seek function to adjust variable *xbare* until a quantity called *cotan eqn* (see Section 2.2) iterates to zero (typically, iteration stops when *cotan eqn* reaches ~ 10^{-5}). The bare critical radius and mass are then computed. For (ii), the user enters in addition the density, atomic weight, elastic-scattering cross-section, and outer radius of the tamper. In a second block of cells labeled *Tamped Threshold Criticality* the user again employs the Goal Seek function to adjust variable *Rtampthresh* until a second version of *cotan eqn* [equation (2.43) Section 2.3] iterates to zero. The tamped threshold critical radius and mass are then computed, as is the mass of the tamper given the specified outer radius. Finally, the user can specify the mass of an *untamped* fissile core; this

should exceed the threshold untamped mass computed in (i); one must also specify the gas/radiation constant γ, the average energy of fission neutrons (in MeV), and the number of "initial" neutrons. Then in a third block of cells, *Untamped Multiple-Mass Efficiency and Yield (Supercriticality)*, the user again invokes the Goal Seek function, this time adjusting *alphaun* until a third version of *cotan eqn* iterates to zero. The calculations of Section 2.4 are then carried out: the criticality and efficiency timescales are computed, as are the efficiency, yield, and pressure at the time of second criticality. All user-input variables are gathered in one block near the top of the spreadsheet in **bold red**. Quantities to be adjusted with Goal Seek appear in regular red type; the quantities to be adjusted to zero appear in **bold green**.

CriticalityNumerical Time-dependent simulation of conditions inside an expanding tamped supercritical core. Consists of three Sheets. Sheet 1 is essentially a duplicate of CriticalityAnalytic above; the user enters the same data and performs the same three Goal Seek operations. Sheet 2 consists of 28 values of the core radius. For each, the user runs Goal Seek, adjusting the value of the exponential criticality parameter α to satisfy the tamped criticality equation (2.44); this is to investigate whether it is sensible to treat α as a linear function of radius. Assuming so, the linear-fit slope and intercept are automatically computed and transferred to sheet 3, where the time-dependent simulation itself is performed. Here, the user need only set the "initial" and "later" timesteps. As programmed, the initial timestep applies only for the first timestep of the simulation following $t = 0$, then the later timestep is used. Adjust the "late" timestep until α is just reaching zero at row 500. Graphs of alpha, yield, log(fission rate), and log(pressure) are automatically generated.

PreDetonation For calculating the predetonation probability of a core that contains a spontaneously fissioning contaminant. User enters core mass, contaminant mass, mass density of core, fission and elastic-scattering cross sections of main core material (e.g., U-235 or Pu-239), number of neutrons emitted per spontaneous fission, spontaneous-fission half-life of contaminant (in years), atomic masses of core and contaminant material, assembly time (microsec), and maximum number of scatterings permitted. The main result is the % probability of non-predetonation. When downloaded, the values entered are for a 64-kg U-235 core containing 20% U-238.

This spreadsheet has been modified (August 2010) from what is described in the book. In the version described in the book, the spreadsheet had two sheets, where Sheet 2 did the calculation of the spherical-core neutron average escape probability as described in Appendix F. However, it has been pointed out to me by Steve Croft of LANL that this calculation can be done analytically: see his paper "The

Distribution of Emergent Flight Path Lengths from Homogeneous Spheres," *Nuclear Instruments and Methods in Physics* **A288**, 589-592 (1990). This is now incorporated in the spreadsheet, making it faster and a bit more accurate. On running the numbers quoted in the book, there is no difference to the predetonation probabilities to the 0.1% level.

Reactor   Simulation of time-dependent evolution of U-235, U-236, U-238, Pu-239, Pu-240, Pu-241, Pu-242 and "fission products" inside a reactor. The user specifies the relevant absorption and fission cross-sections, the thermal power of the reactor (in MW), the number of metric tons of fuel, the timestep in days, the energy per fission in MeV, and the initial number fraction of U-235 in the fuel. The number fraction of each isotope is tracked, as is the cumulative production of Pu (in kg; all 4 isotopes), and the percentage of Pu production that is Pu-239 and Pu-240. A graph of the percentage of Pu that is Pu-240 vs. burnup in MWd/MT is presented. If parameters are changed, it may be necessary to reset graph scales for convenience.

TwoBody   Momentum and energy conservation in a head-on nuclear reaction of the form A + B → C + D as described in Appendix C. Nuclide B is assumed to be stationary when struck by A. User enters nucleon numbers A and Δ-values (MeV) for each nuclide, and the kinetic energy of nuclide A (in MeV). The rest masses are computed (MeV/c^2), as is the Q-value of the reaction. Both possible solutions for the kinetic energies and momenta of C and D are computed, along with indications of whether the solutions are physically valid or not. The threshold value of the kinetic energy of A is also computed, but this should be disregarded if $Q > 0$.

TwoBodyGamma   Momentum and energy conservation in a head-on nuclear reaction of the form A + B → C + γ as described in Appendix D. Nuclide B is assumed to be stationary when struck by A. User enters nucleon numbers A and Δ-values (MeV) for nuclides A, B, C, and the kinetic energy of nuclide A (in MeV). The rest masses are computed (MeV/c^2). Both possible solutions for the energy of the gamma-ray and the kinetic energy and momentum of C are computed, along with "check values" for the kinetic energy of C so that the user can determine which solution(s) is physically valid.

TwoSphereFission Assumes a fission reaction of the form n + A → B + C + N(n), where n represents a neutron. B is the "heavy" fission product and C the "light". The user enters the nucleon numbers and delta values for A, B, and C (and for the neutrons, $A = 1$, and $\Delta = 8.071$) and the number of neutrons produced, N. The program computes the Q-value of the reaction, the mass ratio of the fission products (B/C), the surface energy parameter a_S,

and the limiting value of Z^2/A against spontaneous fission, $Z^2/A = (3.356 \ a_S)$ as described in Section 1.7.

ReflectedCore This spreadsheet was added after the book was published and is very similar to **CriticalityAnalytic** above but with one important change: Here the user specifies a subcritical core mass and the program seeks the tamper outer radius that will just render the core threshold critical. No efficiency calculations are performed here. The untamped criticality calculation is identical to that in **CriticalityAnalytic**. As posted on the website the calculation is done for a 25-kg U-235 core plus tungsten-carbide tamper.