MODELING THE CONSECUTIVE REACTION $A \rightarrow B \rightarrow C$

DIRECTIONS FOR ROLLING THE DICE:

1. Count out 10 die
2. Set up a table on your paper with 3 columns labeled “A,” “B,” and “C”
3. Decide where you are going to place the three piles of die on the table
4. Record initial number of die in each section. (10 in A, 0 in B and 0 in C)
5. Roll the die in A
6. Move any die with a 5 into B
7. Roll the die in B
8. Move any die with a 6 into C
9. Count the number of die in each section and record in your table. This set of data represents one unit of time in the reaction sequence.
10. Repeat steps 5-9 until all die have made it into C
11. Repeat steps 1-10 with 50 and 198 die if time permits.
CREATING AN EXCEL SPREADSHEET FOR THE DATA:

The excel spreadsheet that you will be using has already been set-up. However, if you need to set-up a spreadsheet in the future here are some helpful tips.

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>[A]i</td>
<td>??</td>
<td>k1=</td>
<td>??</td>
<td>k2=</td>
<td>??</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>time</td>
<td>A</td>
<td>B</td>
<td>C</td>
<td>[A] fit</td>
<td>[B] fit</td>
<td>[C] fit</td>
</tr>
</tbody>
</table>

1. In columns A-D put your data in exactly as you have recorded it during the experiment
2. Enter the formulas for fitting the data into E4-G4 for the respective species
   To use the same value from a cell in each equation be sure to put ‘$’ before each reference. The equation for fitting species A that you would put into cell E4 would look like:

\[ =C1\exp(-F1*A4) \]

3. After putting in all of the formulas click the cell once and put your cursor over the box that is on the lower right-hand corner and drag down to fill the remaining cells

Formulas for fitting the data:

\[ [A]_t = [A]_0 \exp(-k_1 t) \]

\[ [B]_t = \frac{k_1}{k_2 - k_1} [A]_0 \left( \exp(-k_1 t) - \exp(-k_2 t) \right) \]

\[ [C]_t = [A]_0 \left( 1 - \frac{k_1}{k_2 - k_1} \left( \exp(-k_1 t) - \exp(-k_2 t) \right) - \exp(-k_1 t) \right) \]
DIRECTIONS FOR PUTTING RANDOM NUMBERS INTO EXCEL:
1. Type the location of the cell that you want to use as your base number
2. Type a ‘+’
3. Type the amount of noise that you want to have associated with your number
4. Type in parenthesis Rand()
5.Followed ‘-‘ and type the range of variation you want around your number

For example to get the random number associated with the data I obtained for the A species in your reactions I typed:

=B4+30*(Rand()-0.5)