A beaker contains three types of molecules, called monomers, dimers, and trimers. We use M, D, and T to stand for the quantities of each of the three respective types. Suppose these quantities are changing over time, according to the following "rate equations:"

$$\begin{aligned} M' &= -4M^2 - 0.8MD, \\ D' &= \quad 2M^2 - 0.8MD, \\ T' &= \qquad\qquad 0.8MD. \end{aligned}$$

Let's suppose that, *initially, there are equal* (nonzero) *quantities of monomers and dimers.*

1. Is D initially increasing or decreasing? Please explain.

   Initially, we have $D = M$, by the above note. So initially, by the above equation for D', we have

   $$\begin{aligned} D' &= 2M^2 - 0.8MD \\ &= 2M^2 - 0.8M \cdot M \\ &= 2M^2 - 0.8M^2 \\ &= (2 - 0.8)M^2 = 1.2M^2 > 0. \end{aligned}$$

   Since D' is initially positive, we see that D is initially increasing.

2. What is the "threshold value" of M/D, meaning the value of the ratio M/D at which D changes from increasing to decreasing (if D is initially increasing), or from decreasing to increasing (if D is initially decreasing)? Please explain.

   To say that D changes from increase to decrease, or vice versa, is to say that $D' = 0$. Let's examine where this happens, by setting the above formula for D' equal to zero:

   $$2M^2 - 0.8MD = 0.$$

   Factor out an M:

   $$M(2M - 0.8D) = 0.$$

   Divide through by M (assuming $M \neq 0$):

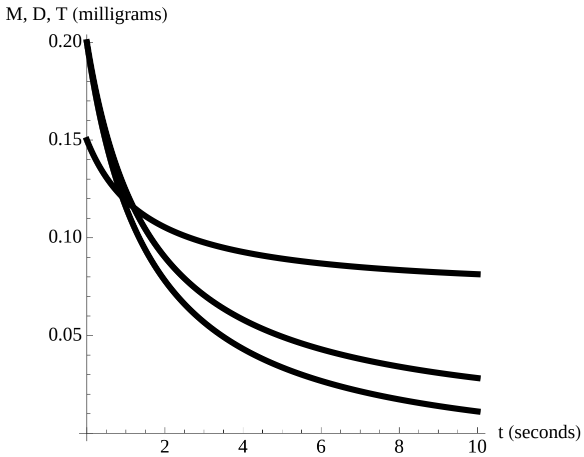
   $$2M - 0.8D = 0.$$

   Solve for M/D:

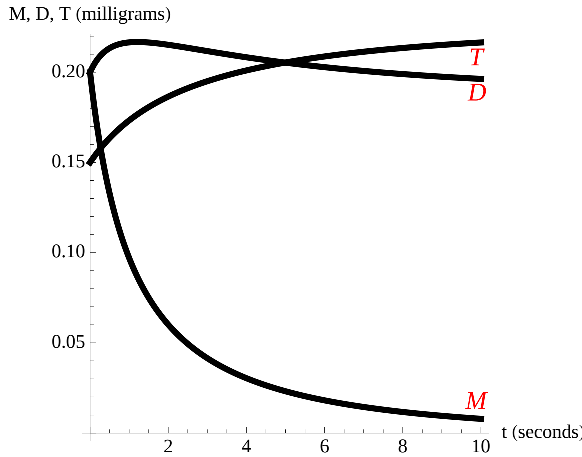
   $$M/D = 0.8/2 = 0.4.$$

   So the threshold value of M/D is 0.4.

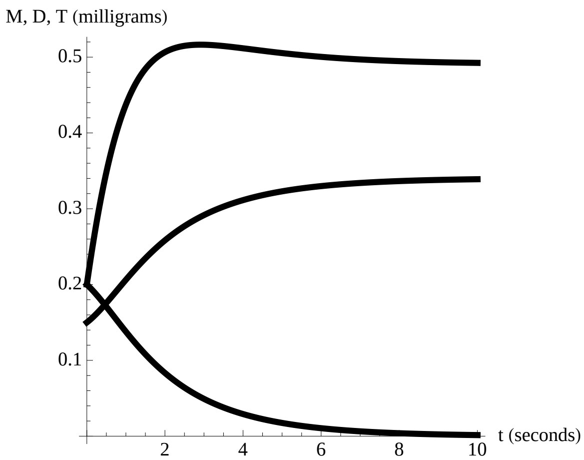
3. Which of the four graphs on the following page could possibly be a graph of the quantities M, D, and T modeled by the above rate equations? Please explain your reasoning carefully, and on the correct graph, label which curve is M, which is D, and which is T. Hint: start by thinking about increase and decrease.



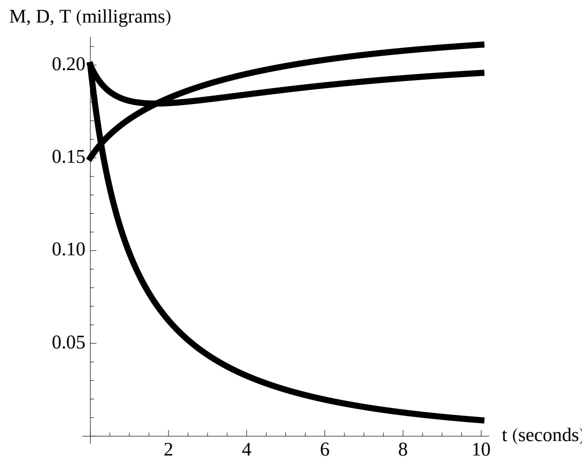
(i)



(ii)



(iii)



(iv)

Since $T' = 0.8MD$ is always positive (as long as neither M nor D equals zero), at least one of our three curves must be steadily increasing. This eliminates graph (i). We can also eliminate graph (iv) because, by exercise 2 above, D' must also increase initially, and graph (iv) does not include two curves that are initially increasing.

To distinguish between graphs (ii) and (iii) we note that, by exercise 2 above, D peaks when M/D equals 0.4. This clearly eliminates graph (iii) – in that graph, at the point (around $t = 2.5$) where D peaks, we see that M is less than 0.1 and D is larger than 0.5, so that M/D is less than $0.1/0.5 = 1/5 = 0.2$.

The remaining graph (ii) must therefore be the correct graph. The labeling of each of the quantities M, D, and T in that graph follows by considering the signs of M', D', and T'.

4. Fill in the blanks (try to answer based primarily on quantitative reasoning and mathematics; you shouldn't need any advanced knowledge of chemical reactions):

   A monomer may react with another monomer to form a dimer. These monomer-to-monomer reactions cause a decrease in the total quantity of ___monomers___. Moreover, the rate at which this occurs is proportional to M^2 (since each of the M milligrams of monomers present has roughly M milligrams of other ___monomers___ with which to react). The monomer-to-monomer reactions therefore correspond to the term ___$-4M^2$___ in the above equation for M'.

   Further, whenever two monomers are lost to a monomer-to-monomer reaction, one ___dimer___ is gained. That is: the rate at which dimers are gained from such reactions equals half the rate at which___monomers___ are lost to these reactions. Since half of $4M^2$ equals ___$2M^2$___, the monomer-to-monomer reactions account for the term ___$2M^2$___ in the above equation for D'.

   A monomer may also react with a dimer to form a ___trimer___. The rate at which this occurs is proportional to the product of the quantity of monomers and the quantity of dimers (since each of the ___M___ milligrams of monomers present has ___D___ milligrams of dimers with which to react). The decrease in M resulting from these monomer-to-dimer reactions therefore corresponds to the term ___$-0.8MD$___ in the above equation for M'. Analogously, the decrease in D resulting from these monomer-to-dimer reactions corresponds to the term ___$-0.8MD$___ in the above equation for D'.

   Finally, when a monomer and a dimer are lost to a monomer-to-dimer reaction, one ___trimer___ is gained. This accounts for the term ___$0.8MD$___ in the above equation for T'.

5. Use the rate equations on the first page, above, to compute $M' + 2D' + 3T'$. What does this tell you about $M + 2D + 3T$? How would you interpret this result in terms of the chemical reactions taking place?

   We readily compute that

$$\begin{aligned} M' + 2D' + 3T' &= -4M^2 - 0.8MD + 2(2M^2 - 0.8MD) + 3(0.8MD) \\ &= (-4 + 2 \cdot 2)M^2 + (-0.8 + 2(-0.8) + 3(0.8))MD \\ &= 0. \end{aligned}$$

   The fact that $M' + 2D' + 3T' = 0$ tells us that $M + 2D + 3T$ is constant.

   Interpretation: if a monomer is considered a basic unit, a dimer counts as two such units, and a trimer counts as three, then the number of basic units is preserved throughout the reaction. (Or to put it another way: no "mers" are created or destroyed!)

6. Show that, in the situation at hand (that is, for the rate equations given at the top of this project), the ratio M/D is *always* decreasing. Hint: use the quotient rule to express $(M/D)'$ in terms of M, D, M', and D'; then use the given rate equations to rewrite your result in terms of M and D only.

   We have

$$\begin{aligned}
\left(\frac{M}{D}\right)' &= \frac{DM' - MD'}{D^2} \\
&= \frac{D(-4M^2 - 0.8MD) - M(2M^2 - 0.8MD)}{D^2} \\
&= \frac{-4M^2D - 0.8MD^2 - 2M^3 + 0.8M^2D}{D^2} \\
&= \frac{(-4 + 0.8)M^2D - 0.8MD^2 - 2M^3}{D^2} \\
&= \frac{-3.2M^2D - 0.8MD^2 - 2M^3}{D^2},
\end{aligned}$$

   which is negative because each summand in the numerator is negative, while the denominator is positive. Since $(M/D)'$ is negative, M/D is decreasing, and we're done.