Calculus I Project: Monomers, Dimers, Trimers, and Rates of Change

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:”

\[
\begin{align*}
M' &= -4M^2 - 0.8MD, \\
D' &= 2M^2 - 0.8MD, \\
T' &= 0.8MD.
\end{align*}
\]

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

\[
D' = 2M^2 - 0.8MD
= 2M^2 - 0.8M \cdot M
= 2M^2 - 0.8M^2
= (2 - 0.8)M^2 = 1.2M^2 > 0.
\]

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.
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

$$ M' + 2D' + 3T' = -4M^2 - 0.8MD + 2(2M^2 - 0.8MD) + 3(0.8MD) $$
$$ = (-4 + 2 \cdot 2)M^2 + (-0.8 + 2(-0.8) + 3(0.8))MD $$
$$ = 0. $$

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

\[
\left( \frac{M}{D} \right)' = \frac{DM' - MD'}{D^2}
\]

\[
= \frac{D(-4M^2 - 0.8MD) - M(2M^2 - 0.8MD)}{D^2}
\]

\[
= \frac{-4M^2D - 0.8MD^2 - 2M^3 + 0.8M^2D}{D^2}
\]

\[
= \frac{(-4 + 0.8)M^2D - 0.8MD^2 - 2M^3}{D^2}
\]

\[
= \frac{-3.2M^2D - 0.8MD^2 - 2M^3}{D^2},
\]

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.