MATHEMATICAL MODELING

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1. Functions

If one agrees that set theory is an appealing foundation of mathematics, then all mathematical objects must be defined as sets of some sort. (Wiki: ordered pair)

1.1. **Function.**

Definition 1.1 (Ordered Pair): *The* ordered pair *of two elements a of a set $\mathcal{S}$ and b of a set $\mathcal{T}$, (a, b), is the set* $(a, b) \equiv \{\{a\}, \{a, b\}\}$ *. Call a the* first component *and b the* second component *of (a, b), respectively.*

Note 1. *If $\mathcal{S}$ is a proper subset of $\mathcal{T}$, then the elements a and b need not be necessarily distinct.*

Note 2. *Two ordered pairs are equal if and only if their correspondent first components* and *second components are equal. That is* [1], $(a, b) = (c, d) \iff a = c \wedge b = d$.

Definition 1.2 (Cartesian Product): *The* Cartesian product *of the sets $\mathcal{S}$ and $\mathcal{T}$, $\mathcal{S} \odot \mathcal{T}$, is the set of all ordered pairs between $\mathcal{S}$ and $\mathcal{T}$;* i.e., $\mathcal{S} \odot \mathcal{T} \equiv \{(a, b) \mid a \in \mathcal{S} \wedge b \in \mathcal{T}\}$.

Note 3. *The Cartesian product does not commute and is generally not associative.*

Definition 1.3 (Function): *A function f from a set $\mathcal{S}$ to a set $\mathcal{T}$ is a subset of the Cartesian product between $\mathcal{S}$ and $\mathcal{T}$, such that every element of $\mathcal{S}$ is the first component of one and only one ordered pair in the subset* [2]*. That is,* $(x, y) \in f \wedge (x, z) \in f \implies y = z$.

Call y the value of f at x, $y = f(x)$*. Call $\mathcal{S}$ the* domain (or source) of f, $D(f)$*, and $\mathcal{T}$ the* codomain (or target) of f, $C(f)$*. Call the subset of all the y elements of the pairs (x, y) the* range of f, $R(f)$.

Notation 1. *A* function f of one real variable *is a function whose domain is a subset of* $\mathbb{R}$*;* i.e., $D(f) \subset \mathbb{R}$.

Notation 2. *A* function f of two variables *is a function whose domain is a subset of the Cartesian product of two sets $\mathcal{A}$ and $\mathcal{B}$;* i.e., $D(f) \subset \mathcal{A} \odot \mathcal{B}$*. Denote the function values by $f(a, b)$ instead of $f((a, b))$.*

Notation 3. *A* function f of two real variables *is a function whose domain is a subset of* $\mathbb{R} \odot \mathbb{R}$.

Notation 4. *A function with domain $\mathcal{D}$ is* defined on a set $\mathcal{S}$ *if $\mathcal{S}$ is a subset of $\mathcal{D}$. If $x \in \mathcal{S}$, call the set of $f(x)$ the* image of $\mathcal{S}$ under f*, denoted $f(\mathcal{S})$. If $\mathcal{T}$ is any set which contains $f(\mathcal{S})$, then f is also called* mapping from $\mathcal{S}$ to $\mathcal{T}$*, denoted $f\colon \mathcal{S} \to \mathcal{T}$. If $f(\mathcal{S}) = \mathcal{T}$, then the mapping is said to be* onto $\mathcal{T}$*. A mapping of $\mathcal{S}$ into itself is sometimes called a* transformation.

Date: March 10, 2013.

Key words and phrases. mathematical modeling index notation engineering.

[1] The symbols $\iff$ and $\wedge$ mean "if and only if" and "logical and", respectively.

[2] Or, [...] such that for *every* element of $\mathcal{S}$ there is a *unique* element of $\mathcal{T}$.

NOTATION 5. *The following notation is also used for denoting functions*

$$\begin{aligned} f \,:\, \mathcal{S} &\to \mathcal{T} \\ x &\mapsto f(x)\,. \end{aligned}$$

This is read: "f is a function from the set $\mathcal{S}$ to the set $\mathcal{T}$ that maps x in $\mathcal{S}$ to $f(x)$ in $\mathcal{T}$".

NOTATION 6. *The notation $f(x) = \dots$ is used when the domain and codomain of f are known or understood and the value of f at x is given by a formula;* e.g., $f(x) = ax^2 + bx + c$.

NOTE 4. *Instead of describing a function f by specifying explicitly the pairs it contains, it is preferable to describe the domain of f and then, for each x in $D(f)$, to describe how the function value $f(x)$ is obtained.*

DEFINITION 1.4 (Constant Function): *A* constant function *is a function whose range consists of a single number.*

DEFINITION 1.5 (Linear Function): *A* linear function *is a function g defined for all real x by a formula of the form $g(x) = ax + b$.*

DEFINITION 1.6: *Consider two real functions f and g having the same domain $\mathcal{D}$. Construct the following functions for all x in $\mathcal{D}$*

- ⋄ *sum of f and g, $f + g$: $u(x) = f(x) + g(x)$,*
- ⋄ *product of f and g, $f \cdot g$: $v(x) = f(x) \cdot g(x)$,*
- ⋄ *quotient of f and g, f/g: $w(x) = f(x)\,/g(x)$, if $g(x) \neq 0$.*

EXAMPLE 1.1. Express the quadratic equation $ax^2 + bx + c$ as a map.

Solution.

$$\begin{aligned} f \,:\, \mathbb{R} &\to \mathbb{R} \\ x &\mapsto ax^2 + bx + c, \end{aligned}$$

where a, b and c are constant real numbers. Sometimes this map is simply written $f(x) = ax^2 + bx + c$. □

EXAMPLE 1.2. Define a *binary operation*.

Solution. A binary operation $*$ on a set $\mathcal{M}$ is a map

$$\begin{aligned} \mathcal{M} \odot \mathcal{M} &\to \mathcal{M} \\ (x, y) &\mapsto x * y\,. \end{aligned}$$

A binary operation is also called a binary transformation or a binary composition. □

REMARK 1. *A* binary *operation is a function with two variables, thus the Cartesian product and the ordered pair. Note also that binary operations are closed: the Cartesian product is rather a Cartesian power (Cartesian product over the same set) and the map is onto itself, thus it could be called a transformation.*

1.2. **Area.** Definition of area: [**?** , p. 57].

DEFINITION 1.7 (Set Function): *A* set function *is a function whose domain is a collection of sets and whose function values are real numbers.*

DEFINITION 1.8 (Measurable Set): *A* measurable set *is a set to which an area can be assigned.*

Definition 1.9 (Congruence): *Two sets are said to be congruent if their points can be put into one-to-one correspondence in such a way that distances are preserved;* i.e., *if two points $\mathcal{P}$ and $\mathcal{Q}$ in one set correspond to $\mathcal{P}'$ to $\mathcal{Q}'$ in the other, then the distance from $\mathcal{P}$ to $\mathcal{Q}$ must be the same as the distance from $\mathcal{P}'$ to $\mathcal{Q}'$; this must be true for all choices of $\mathcal{P}$ and $\mathcal{Q}$.*

Definition 1.10 (Rectangle): *A* rectangle *is any set congruent to a set of the form*

$$\{(x, y) \mid 0 \leq x \leq h, 0 \leq y \leq k\} ,$$

where $h \geq 0$ and $k \geq 0$. The numbers h and k are called the lengths of the edges of the rectangle.

Note 5. *We consider a line segment or a point to be the special case of a rectangle by allowing h or k (or both) to be zero.*

Definition 1.11 (Step Region): *A* step region *is the union of a finite collection of adjacent rectangles with their bases resting on the x-axis.*

Definition 1.12 (Ordinate Set): *An* ordinate set *is a graph whose upper boundary is the graph of a nonnegative function.*

Motivation: When we assign an area to a plane region, we associate a number with a set $\mathcal{S}$ in the plane. From a purely mathematical viewpoint, this means that we have a function a (an area function) which assigns a real number $a(\mathcal{S})$ (the area of $\mathcal{S}$) to each set $\mathcal{S}$ in some given collection of sets [3]. That is, area is a set function. The basic problem is this: given a plane set $\mathcal{S}$, what area $a(\mathcal{S})$ shall we assign to $\mathcal{S}$?

Our approach is to start with a number of properties we feel area should have and take this as *axioms* for area. Any set function that satisfies these axioms will be called an area function. (It has to be proven that an area function exists, so not to develop an empty theory! Not done here ;(

Remarks about the collection of sets in the plane to which an area can be assigned. These sets will be called *measurable sets*; the collection of all the measurable sets will be denoted by $\mathfrak{M}$. The axioms contain enough information about the sets in $\mathfrak{M}$ to allow us to prove that all the geometric figures arising in the usual applications of calculus are in $\mathfrak{M}$ and their areas can be calculated by integration.

One of the axioms (Axiom 5) states that every rectangle is measurable and its area is the product of the lengths of its edges.

From rectangles we can build up more complicated sets, such as step regions. The axioms imply that each step region is measurable and that its area is the sum of the areas of the rectangular pieces.

Axiom 6 will enable to prove that many ordinate sets are measurable and that their areas can be calculated by approximating such sets by inner or outer step regions.

Axiom 1.1 (Axiomatic Definition of Area): *We assume there exists a class $\mathfrak{M}$ of measurable sets in the plane and a set function a, whose domain is in $\mathfrak{M}$, with the following properties*

1. *Nonnegative property: for each set $\mathcal{S}$ in $\mathfrak{M}$, we have $a(\mathcal{S}) \geq 0$.*
2. *Additive property: if $\mathcal{S}$ and $\mathcal{T}$ are in $\mathfrak{M}$, then $\mathcal{S} \cup \mathcal{T}$ and $\mathcal{S} \cap \mathcal{T}$ are in $\mathfrak{M}$, and we have $a(\mathcal{S} \cup \mathcal{T}) = a(\mathcal{S}) + a(\mathcal{T}) - a(\mathcal{S} \cap \mathcal{T})$.*
3. *Difference property: if set $\mathcal{S}$ and $\mathcal{T}$ are in $\mathfrak{M}$ with $\mathcal{S} \subseteq \mathcal{T}$, then $\mathcal{T} - \mathcal{S}$ is in $\mathfrak{M}$, and we have $a(\mathcal{T} - \mathcal{S}) = a(\mathcal{T}) - a(\mathcal{S})$.*
4. *Invariance under congruence: if a set $\mathcal{S}$ is in $\mathfrak{M}$ and if $\mathcal{T}$ is congruent to $\mathcal{S}$, then $\mathcal{T}$ is also in $\mathfrak{M}$ and we have $a(\mathcal{S}) = a(\mathcal{T})$.*

[3] In the definition of volume, this collection is called a class. Moreover, the collection should be a collection of measurable sets.

(5) *Choice of scale: every rectangle $\mathcal{R}$ is in $\mathfrak{M}$. If the edges of $\mathcal{R}$ have lengths h and k, then $a(\mathcal{R}) = hk$.*
(6) *Exhaustion property: let $\mathcal{Q}$ be a set that can be enclosed between two step regions $\mathcal{S}$ and $\mathcal{T}$, so that*

$$\mathcal{S} \subseteq \mathcal{Q} \subseteq \mathcal{T}. \tag{1}$$

If there is only one number c that satisfies the inequalities

$$a(\mathcal{S}) \leq c \leq a(\mathcal{T})$$

for all step regions $\mathcal{S}$ and $\mathcal{T}$ satisfying **??**, *then $\mathcal{Q}$ is measurable and $a(\mathcal{Q}) = c$.*

Axiom 3 implies that $\emptyset$ is measurable and has zero area. Since $a(\mathcal{T} - \mathcal{S}) \geq 0$, Axiom 3 also implies the *monotone property*

$$a(\mathcal{S}) \leq a(\mathcal{T})$$

for sets $\mathcal{S}$ and $\mathcal{T}$ in $\mathfrak{M}$ with $\mathcal{S} \subseteq \mathcal{T}$. In other words, a set which is part of another cannot have a larger area.

Axiom 4 assigns equal areas to sets that have the same size and shape. Axiom 5 assigns a nonzero area to some rectangles and thus excludes the trivial case of assigning the real zero as the area of every set in $\mathfrak{M}$.

Finally, repeated use of the additive property shows that every step region is measurable and that its area is the sum of the areas of the rectangular pieces.

1.3. **Volume.** Definition of volume: [**?** , p. 115].

Motivation: We assume there exist certain sets $\mathcal{S}$ of points in three-dimensional space, which we call *measurable sets*, and a set function v, called a *volume function*, which assigns to each measurable set $\mathcal{S}$ a number $v(\mathcal{S})$, called the volume of $\mathcal{S}$. We use the symbol $\mathfrak{A}$ to denote the class of all measurable sets in three-dimensional space, and we call each set $\mathcal{S}$ in $\mathfrak{A}$ a *solid*.

We list a number of properties that we like the volume to have and take them as the axioms for volume. The choice of axioms will allow us to prove that the volumes of many solids can be computed by integration.

The first three axioms describe the nonnegative, additive and difference properties. We use the principle called *Cavalieri's principle* that assigns equal volumes to congruent solids which, though not congruent, have equal cross-sectional areas cut by planes perpendicular to a given line. More precisely, suppose $\mathcal{S}$ is a given solid and $\mathcal{L}$ a given line. If a plane $\mathcal{F}$ is perpendicular to $\mathcal{L}$, the intersection $\mathcal{F} \cap \mathcal{L}$ is called a cross-sectional perpendicular to $\mathcal{L}$. If every cross-sectional perpendicular to $\mathcal{L}$ is a measurable set in its own plane, we call $\mathcal{S}$ a *Cavalieri solid*. Cavalieri's principle assigns equal volumes to two Cavalieri solids, $\mathcal{S}$ and $\mathcal{T}$, if $a(\mathcal{S} \cap \mathcal{T}) = a(\mathcal{T} \cup \mathcal{S})$ for every plane $\mathcal{F}$ perpendicular to a given line $\mathcal{L}$.

The next axioms states that the volume of a parallelepiped is the product of the length of its edges. A rectangular parallelepiped is any set congruent to a set of the form

$$\{(x, y, z) \mid 0 \leq x \leq a, 0 \leq y \leq b, 0 \leq z \leq c\} .$$

We shall use the term *box* instead of rectangular parallelepiped. The nonnegative numbers a, b, c are called the lengths of the edges of the box.

Finally, we include an axiom that states that every convex set is measurable. A set is called *convex* if, for every pair of points $\mathcal{P}$ and $\mathcal{Q}$ in the set, the line segment joining $\mathcal{P}$ and $\mathcal{Q}$ is also in the set. This axiom, along with the additive and difference properties, ensures that all the elementary solids that occur in usual applications of calculus are measurable.

Axiom 1.2 (Axiomatic Definition of Volume): *We assume there is a class* [4] $\mathfrak{A}$ *of solids and a set function v, whose domain is in $\mathfrak{A}$, with the following properties:*

[4] A class is a collection of sets; *i.e.*, a set of sets.

(1) *Nonnegative property: for each set $\mathcal{S}$ we have $v(\mathcal{S}) \geq 0$.*
(2) *Additive property: If $\mathcal{S}$ and $\mathcal{T}$ are in $\mathfrak{A}$, then $\mathcal{S} \cup \mathcal{T}$ and $\mathcal{S} \cap \mathcal{T}$ are in $\mathfrak{A}$, and we have*
$$v(\mathcal{S} \cup \mathcal{T}) = v(\mathcal{S}) + v(\mathcal{T}) - v(\mathcal{S} \cap \mathcal{T}) \ .$$
(3) *Difference property: if $\mathcal{S}$ and $\mathcal{T}$ are in $\mathfrak{A}$ with $\mathcal{S} \subseteq \mathcal{T}$, then $\mathcal{T} - \mathcal{S}$ is in $\mathfrak{A}$, and we have*
$$v(\mathcal{T} - \mathcal{S}) = v(\mathcal{T}) - v(\mathcal{S}) \ .$$
(4) *Cavalieri's principle: if $\mathcal{S}$ and $\mathcal{T}$ are two Cavalieri solids in $\mathfrak{A}$ with $a(\mathcal{S} \cap \mathcal{F}) \leq a(\mathcal{T} \cap \mathcal{F})$ for every plane $\mathcal{F}$ perpendicular to a given line, then $v(\mathcal{S}) \leq v(\mathcal{T})$.*
(5) *Choice of scale: every box $\mathcal{B}$ is in $\mathfrak{A}$. If the edges of $\mathcal{B}$ have lengths a, b and c, then $v(\mathcal{B}) = abc$.*
(6) *Every convex set is in $\mathfrak{A}$.*

NOTE 6. *Axiom 3 shows that the empty set $\emptyset$ is in $\mathfrak{A}$ and has zero volume. Axiom 3 also implies the following monotone property:*
$$v(\mathcal{S}) \leq v(\mathcal{T}) \,,$$
for sets $\mathcal{S}$ and $\mathcal{T}$ in $\mathfrak{A}$ with $\mathcal{S} \subseteq \mathcal{T}$.

1.4. **Work.** Definition of work: [**?** , p. 115].

Motivation: Work is a measure of the energy expended by a force in moving a particle from one point to another. In this section we consider linear motion. That is, we assume that the motion takes place along a line (x-axis) from one point, say $x = a$, to another point, $x = b$, and we also assume that the force acts along this line. We assume further that the force acting on the particle is a function of position. If the particle is at x, we denote the force by $f(x)$ the force acting on it, where $f(x) > 0$ if the force acts in the direction of the positive x-axis and $f(x) < 0$ if the force acts in the opposite direction. When the force is constant, say $f(x)$ for all x between a and b, we define the work done by f to be the number $c \cdot (b - a)$, *i.e.*, force times displacement. The work may be positive or negative.

If force is measured in N and distance in m, then we measure work in N m or J.

Now, suppose the force is not necessarily constant but is a given function of position defined on the interval joining a and b. How do we define the work done by f in moving a particle from a to b? We state some properties of work dictated by physical requirements. Then we prove that for any definition of work with these properties, the work done by the integrable force function f is equal to the integral $\int_a^b f(x)\ dx$.

DEFINITION 1.13 (Fundamental Properties of Work): *Let $W_a^b(f)$ denote the work done by a force function f in moving a particle from a to b. Then, work has the following properties:*
(1) *additive property: if $a < c < b$, then $W_a^b(f) = W_a^c(f) + W_c^b(f)$.*
(2) *monotone property: if $f \leq g$ on $[a, b]$, then $W_a^b(f) \leq W_a^b(g)$. That is, a greater force does greater work.*
(3) *elementary formula: if f is constant, say $f(x) = c$ for all x in the open interval $]a, b[$, then $W_a^b(f) = c \cdot (b - a)$.*

The additive property can be extended by mathematical induction to any finite number of intervals; *i.e.*, if $a = x_0 < \cdots < x_n = b$, we have
$$W_a^b(f) = \sum_{k=1}^{n} W_k \,,$$
where W_k is the work done by f from x_{k-1} to x_k. In particular, if the force is a step function s which takes a constant value s_k on the open interval $]x_{k-1}, x_k[$, property 3 states that $W_k =$

$s_k \cdot (x_k - x_{k-1})$, so we have

$$W_a^b(s) = \sum_{k=1}^{n} s_k \cdot (x_k - x_{k-1}) = \int_a^b s(x)\ dx\,.$$

Thus, for step functions, work has been expressed as an integral. This leads to a more general theorem.

THEOREM 1.1: *Suppose work has been defined for a class of force functions f in such a way that it satisfies properties 1, 2 and 3. Then, the work done by an integrable force function moving a particle from a to b is equal to the integral of f,*

$$W_a^b(f) = \int_a^b f(x)\ dx.$$

Proof. Let s and t be two step functions satisfying $s \le f \le t$ on $[a, b]$. The monotone property of work states that $W_a^b(s) \le W_a^b(f) \le W_a^b(t)$. But $W_a^b(s) = \int_a^b s(x)\ dx$ and $W_a^b(t) = \int_a^b t(x)\ dx$, so the number $W_a^b(f)$ satisfies the inequalities

$$\int_a^b s(x)\ dx \le W_a^b(f) \le \int_a^b t(x)\ dx$$

for all the step functions s and t satisfying $s \le f \le t$ on $[a, b]$. Since f is integrable on $[a, b]$, it follows that $W_a^b(f) = \int_a^b f(x)\ dx$. $\square$

NOTE 7. *The additive property of work for step force functions, $W_a^b(s) = \sum_{k=1}^{n} s_k \cdot (x_k - x_{k-1})$, leads to a nice computer software implementation! I think ;)*

2. Material Decay

EXERCISE 2.1. Consider a substance that decays into another one according to the law A $\longrightarrow$ B. Find the number of particles of the decaying substance at any time given that its initial number is $N(0)$.

Solution. Let $\mathbb{R}^+$ denote the set of non-negative real numbers and $\mathcal{I}_{\mathrm{A}}$ the interval $[0, N_{\mathrm{A}}(0)]$. Let A represent the decaying substance, $N_{\mathrm{A}} \in \mathcal{I}_{\mathrm{A}}$ the number of particles of A and $t \in \mathbb{R}^+$ time.

Define a C^1 function $N_{\mathrm{A}} : \mathbb{R}^+ \to \mathcal{I}_{\mathrm{A}}$. Call the function *number of particles of* A. Denote its value at t by $N_{\mathrm{A}}(t)$.

The change of $N_{\mathrm{A}}(t)$ during an interval Δt is

$$\Delta N_{\mathrm{A}}(t) = N_{\mathrm{A}}(t + \Delta t) - N_{\mathrm{A}}(t) \ .$$

Model the decay by assuming the difference quotient of N_{A} proportional to N_{A} at any t; *i.e.*,

$$-\frac{\Delta N_{\mathrm{A}}(t)}{\Delta t} \propto N_{\mathrm{A}}(t) \ .$$

That is,

$$-\frac{\Delta N_{\mathrm{A}}(t)}{\Delta t} = \alpha_{\mathrm{A}} \, N_{\mathrm{A}}(t) \ ,$$

where $\alpha_{\mathrm{A}} \in \mathbb{R}^+$ is a property of A called the *decay constant*.

Apply the definition of the derivative to the difference quotient and use Leibniz notation to find the rate of change of N_{A} at t:

$$-\frac{\mathrm{d}N_{\mathrm{A}}(t)}{\mathrm{d}t} = -\lim_{\Delta t \to 0} \frac{\Delta N_{\mathrm{A}}(t + \Delta t) - N_{\mathrm{A}}(t)}{\Delta t} \, .$$

The material decay model thus becomes a *0-D ordinary differential equation*

$$-\frac{\mathrm{d}N_{\mathrm{A}}(t)}{\mathrm{d}t} = \alpha_{\mathrm{A}} \, N_{\mathrm{A}}(t) \ .$$

Solve the differential equation by standard methods and apply then the *boundary conditions* to find

$$\frac{N_{\mathrm{A}}(t)}{N_{\mathrm{A}}(0)} = \exp(-\alpha_{\mathrm{A}} t) \, .$$

The last expression models the required the particle decay of A at any time. □

Discussion. The standard model for material decay is the empirical observation that the rate at which N_{A} changes is proportional N_{A} present at the same instant. So, the solution of the problem is to work towards mathematically representing this fact.

The solution begins establishing notation and ranges of variables. Time is represented by a non-negative variable that extends to infinity, whereas the number of particles of A by a number confined within an interval: $[0, N_{\mathrm{A}}(0)]$ (remember that an interval is a set of real numbers). This interval is set to satisfy the physical constrain that N_{A} cannot exceed the given initial amount, while A *decays*.

Then, the function N_{A} is defined. Mathematically, N_{A} establishes a relationship between t and N of A: it takes times and relates them to particle numbers [5]. This function is assumed to be differentiable or, equivalently, a C^1 function, [**?** , p. 138]. This assumption guaranties replacing the difference quotient of N_{A} for its derivative, [**?** , p. 159]. Physically, on the other hand, this relation only approximates material decay, because, even though N_{A} is assumed to be C^1, a continuous function, the N_{A} is in reality a discrete function. Physical experimentation decides the correctness of this assumption.

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[5] An amusing way of thinking about how a function works is to “make it talk”! So, N_{A} would say: “give me any time t and I'll give you the numbers of entities of A at that instant”.

The next step is to relate the standard decay model with the function N_{A} via the differential quotient of N_{A}. Then the definition of derivative is applied to N_{A} to find the decay rate of N. The resulting 0-D ordinary differential equation is solved by standard methods and then the boundary conditions applied, given finally the desired model.

3. Concentration

Exercise 3.1. Consider a vessel holding a reactive, homogeneous solution of a solid solute into a liquid solvent. Find concentration of the solute at any time given that its initial mass is $m(0)$.

Solution. Let $\mathcal{I}_\mathrm{s}$ denote the interval $[0, m_\mathrm{s}(0)]$, $\mathbb{R}^+$ the set of non-negative real numbers and $\mathbb{R}^{3^+}$ the set of non-negative real numbers in $\mathbb{R}^3$. Let $\mathcal{V} \subset \mathbb{R}^{3^+}$ represent the volume of the solution, s the solute, $m_\mathrm{s} \in \mathcal{I}_\mathrm{s}$ the mass of s and $t \in \mathbb{R}^+$ time.

Define a C^1 function $m_\mathrm{s} \colon \mathbb{R}^+ \to \mathcal{I}_\mathrm{s}$. Call the function *mass of* s. Denote its value at t by $m_\mathrm{s}(t)$.

Define the interval

$$\mathcal{I}'_\mathrm{s} = [0, m_\mathrm{s}(0) \,/\mathcal{V}] \,.$$

Define a C^1 function $\gamma_\mathrm{s} \colon \mathbb{R}^+ \to \mathcal{I}'_\mathrm{s}$ by the formula

$$\gamma_\mathrm{s}(t) \equiv \frac{m_\mathrm{s}(t)}{\mathcal{V}} \,.$$

Call γ_s *mass concentration of* s.

Thus, $\mathcal{I}'_\mathrm{s}$ is equivalent to $[0, \gamma_\mathrm{s}(0)]$, where $\gamma_\mathrm{s}(0)$ is the initial concentration of s.

□

Based on [**?**].

Consider a vessel holding a non-reactive, heterogeneous solution of a solute s of mass m_s, $m_\mathrm{s} \in \mathbb{R}$, in a liquid solvent.

Denote the volume of the mixture by $\mathcal{V}$, $\mathcal{V} \subset \mathbb{R}^3$, the coordinates of any point $\mathbf{r} \in \mathcal{V}$ by $\left(x^1, x^2, x^3\right)$ and the time of mixing by t, $t \in \mathbb{R}$.

Since the solution is heterogeneous, the mass of s varies from point to point in $\mathcal{V}$; *i.e.*, the mass of s could be considered as a function mapping time and space into real numbers: $m_\mathrm{s} \colon \mathbb{R} \odot \mathcal{V} \to \mathbb{R}$, herein simply referred to as $m_\mathrm{s}(t, \mathbf{x})$.

Define the concentration of s, γ_s, at a point $\mathbf{x}$ and at an instant t by

$$\gamma_\mathrm{s}(t, \mathbf{x}) \equiv \frac{m_\mathrm{s}(t, \mathbf{x})}{\mathcal{V}}.$$

$\langle a \leq b \rangle$