Convection-Diffusion-Reaction Model

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Abstract

This is one of the most frequently used models in science and engineering. It describes how the concentration of one or more substances (e.g., pollutants) distributed in a medium (river) changes under the influence of three processes, namely, convection, diffusion, and reaction. It is a partial differential equation (PDE) that can be derived using the physical law of mass conservation and the mean value theorem of calculus.

Convection refers to the movement of a substance within a medium (e.g., water or air). *Diffusion* is the movement of the substance from an area of high concentration to an area of low concentration, resulting in the uniform distribution of the substance. A chemical *reaction* is a process that results in the interconversion of chemical substances. The Convection-Diffusion-Reaction (CDR) model is a mathematical model that describe how the concentration of the substance distributed in the medium changes under the influence of these three processes.

We first introduce the notation for this model. Note carefully the corresponding physical units. A *dimension* defines some physical characteristics. For example, length $[L]$, mass $[M]$, time $[T]$, velocity $[L/T]$, and force $[N = ML/T^2]$. A *unit* is a standard or reference by which a dimension can be expressed numerically. In SI (the International System of Units or in the French name Systeme Internationale d'Unites), the *meter* $[m]$, *kilogram* $[kg]$, *second* $[s]$, *ampere* $[A]$, *kelvin* $[K]$, and *candela* $[cd]$ are the base units for the six fundamental dimensions of length, mass, time, electric current, temperature, and luminous intensity.

The notation, meaning, and unit of physical quantities for the CDR model are summarized in the following table.

Symbol	Meaning	Unit
Substance	Pollutants, Chemicals, Electrons (Mass)	M
$x \in [a,b] \subset R^1$	Coordinate	L
$t \in [0,T]$	Time	T
$u \equiv u(x,t)$	The density or concentration of a substance at x and at time t.	$\frac{M}{L}$
$v \equiv v(x,t)$	The velocity of the medium in which the substance moves (from left to right).	$\frac{L}{T}$
uv	Convection, Advection, Drift	$\frac{M}{T}$
	Diffusion	$\frac{M}{T}$
$D \equiv D(x)$	Diffusion coefficient (diffusivity of the medium)	$\frac{L^2}{T}$
$f \equiv f(x,t)$	Reaction: The rate at which the density of mass is changing due to source, sink, or reaction.	$\frac{M}{LT}$
$q \equiv q(x,t)$ $= uv - D\frac{\partial u}{\partial x}$	The rate at which the substance passes (flux) through x at time t.	$\frac{M}{T}$

We consider the change of the total mass of the substance in any space interval $[x, x+\Delta x]$ in the medium and in any time interval $[t, t+\Delta t]$. The law of mass conservation implies that

$$\begin{aligned} &\int_x^{x+\Delta x} [u(s,t+\Delta t) - u(s,t)]\, ds \\ &= [q(x,t) - q(x+\Delta x,t)]\, \Delta t + \int_x^{x+\Delta x} [f(s,t)\Delta t]\, ds \end{aligned} \tag{1}$$

where the first integral represents the total mass change in $[x, x+\Delta x]$ during $[t, t+\Delta t]$. It is equal to the sum of the second term (representing the mass difference flowing in and out) and the last integral (representing the creation (or loss) of the substance). Assuming that all functions are continuous in x, the mean value theorem of calculus tells us that there exist $x^* \in [x, x+\Delta x]$ such that

$$
\begin{aligned}
&[u(x^*, t + \Delta t) - u(x^*, t)]\, \Delta x \\
&= [q(x, t) - q(x + \Delta x, t)]\, \Delta t + [f(x^*, t)\Delta t]\, \Delta x
\end{aligned}
\tag{2}
$$

Dividing both sides by $\Delta x \Delta t$, and then passing the limits $\Delta x \to 0$ and $\Delta t \to 0$, we have the following **1D Convection-Diffusion-Reaction Model**

$$
\begin{aligned}
\frac{\partial u}{\partial t} &= -\frac{\partial q}{\partial x} + f(x, t) = -\frac{\partial}{\partial x}(uv - D\frac{\partial u}{\partial x}) + f(x, t) \\
&= D\frac{\partial^2 u}{\partial x^2} - v\frac{\partial u}{\partial x} + f(x, t)
\end{aligned}
\tag{3}
$$

if we assume that the diffusion coefficient D and the velocity v are constants. This is a **parabolic PDE**. The **3D Convection-Diffusion-Reaction Model** is written as

$$
\frac{\partial u}{\partial t} = \nabla \cdot (D\nabla u) - \overrightarrow{v} \cdot \nabla u + f(\mathbf{r}, t) \tag{4}
$$

where

$$
\begin{aligned}
\mathbf{r} &= (x, y, z) \\
\nabla &= (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}) \text{ : the gradient operator,} \\
\nabla \cdot &= \text{div : the divergence operator,} \\
\overrightarrow{v} &= (u, v, w) \text{ : the velocity in 3D.}
\end{aligned}
$$

In steady state the all functions no longer changing with time, i.e. $\frac{\partial u}{\partial t} = 0$, and assuming $\overrightarrow{v} = f = 0$, Eq. (4) then reduces to the **Laplace equation**

$$
\Delta u = 0 \tag{5}
$$

where

$$
\Delta = \nabla \cdot \nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \text{ : the Laplace operator.}
$$

If $f = f(\mathbf{r}) \neq \mathbf{0}$, we have the **Poisson equation** (an **elliptic PDE**)

$$
-\Delta u = f \tag{6}
$$