

CLL110: Transport Phenomena

Lecture Note 1

Department of Chemical Engineering, IIT Delhi
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Vector and Tensor Analysis: Part 1

Introduction

Transport Phenomena is the subject which deals with the movement of different physical quantities in any chemical or mechanical process and describes the basic principles and laws of transport. It also describes the relations and similarities among different types of transport that may occur in any system. Transport in a chemical or mechanical process can be classified into three types:

1. **Momentum transport:** Deals with the transport of momentum in fluids and is also known as fluid dynamics.
2. **Energy transport:** Deals with the transport of different forms of energy in a system and is also known as heat transfer.
3. **Mass transport:** Deals with the transport of various chemical species themselves.

Three different types of physical quantities are used in transport phenomena:

- **Scalars** (e.g. temperature, pressure, and concentration)
- **Vectors** (e.g. velocity, momentum, and force)
- **Second-order tensors** (e.g. stress or momentum flux, and velocity gradient)

It is essential to have a primary knowledge of the mathematical operations of scalar, vector, and tensor quantities for solving the problems of transport phenomena.

Vectors

In contrast, consider the velocity of a particle or element of fluid; to describe it fully, we need to specify both its magnitude (in some suitable units) and its instantaneous spatial direction. Other examples are momentum, heat flux, and mass flux. These quantities are described by vectors.

In books, vectors are printed in boldface. In ordinary writing, we may represent a vector in different ways.

Vector Notation Conventions

- **Gibbs notation:** $\bar{v}, \vec{v}, \underline{v}, v$
- **Index notation:** v_i

In this course, we will be using the following notations for scalar, vector, and tensor quantities:

Notation:

a, b, c	scalar quantities
$\underline{u}, \underline{v}, \underline{w}$	vector quantities
$\underline{\sigma}, \underline{\tau}$	second-order tensor quantities

We represent a vectorial quantity with a symbol, but we often know it only through its components in a given basis set. Note that the vector, as a geometric entity, possesses an **invariant** identity that is independent of the basis set chosen for its representation.

Basis Sets

The most common basis set in three-dimensional space is the orthogonal triad ($\underline{i}, \underline{j}, \underline{k}$) corresponding to a rectangular Cartesian coordinate system. \underline{i} stands for a unit vector in the x- direction and $\underline{j}, \underline{k}$ represent unit vectors in y, z directions respectively. Note that this is not a unique basis set. The directions of $\underline{i}, \underline{j}, \underline{k}$ depend on our choice of the coordinate directions.

There is no reason for the basis set to be composed of orthogonal vectors. The only requirement is that the three vectors chosen do not lie in a plane. Orthogonal sets are the most convenient, however.

In fact, the use of the indicial notation which we will be studying in the next few lectures will enable us to express the long formulae encountered in transport phenomena in a concise and compact fashion.

Tensor quantities

Most of us might have already encountered scalars and vectors in the study of high-school physics. The essential difference between these two, it was pointed out, was that the vectors also have a direction associated with them along with a magnitude, whereas scalars only have a magnitude but no direction. Extending this definition, we can loosely define a 2nd order tensor as a physical quantity which has a magnitude and two different directions associated with it.

To better understand why we might need two different directions for specifying a particular physical quantity, let us take the example of the stresses which may arise in a solid body, or a fluid. Clearly, the stresses are associated with a force, as well as with an area, whose direction is specified by the outward normal to the face on which it is acting. Hence, we will require 3^2 , i.e. 9 components to specify a stress completely. In general, an n th order tensor

will be specified by 3^n components (in a 3-dimensional system¹). However, the number of components alone cannot determine whether a physical quantity is a vector or a tensor. The additional requirement is that there should be a linear transformation rule for obtaining the corresponding tensors if we rotate the coordinate system about the origin. Thus, tensor quantities can be defined by two essential conditions:

1. These quantities should have 3^n components. According to this definition, scalar quantities are zero-order tensors and have $3^0 = 1$ component. Vector quantities are first-order tensors and have $3^1 = 3$ components. Second-order tensors have $3^2 = 9$ components and third-order tensors have $3^3 = 27$ components. Third and higher-order tensors are not used in transport phenomena, and are hence not dealt with here.
2. The second necessary requirement of any tensor quantity is that it should follow some transformation rule for changing coordinate systems, which will be discussed later.

Kronecker Delta & Alternating Unit Tensor

There are two particular tensors which are quite useful in conveniently and concisely expressing several mathematical operations on tensors. These are the Kronecker delta and the Alternating Unit Tensor.

Kronecker delta (δ_{ij})

Kronecker delta or kronecker's delta is a function of two variables, usually integer, which is 1 if they are equal and 0 otherwise.

It is expressed as a symbol δ_{ij}

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$

Thus, in three dimensions, we may also express the Kronecker delta as

$$\delta_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Alternating Unit Tensor (ε_{ijk}) (also known as Levi Civita symbol or Permutation Symbol)

The alternating unit tensor ε_{ijk} is useful when expressing certain results in a compact form in index notation. Since it has three indices, it has $3 \times 3 \times 3$ possible combinations. The

¹In an m -dimensional system, an n^{th} order tensor will have m^n components. In transport phenomena, we deal with 3D systems in general, and hence $m = 3$.

value of these combinations are as follows:

- $\varepsilon_{ijk} = 0$ if any two of indices i, j, k are equal. For example, $\varepsilon_{113}, \varepsilon_{131}, \varepsilon_{111}, \varepsilon_{222} = 0$
- $\varepsilon_{ijk} = +1$ when the indices i, j, k are different and form an even permutation of (123), i.e. are in cyclic order. For example in Fig.1, ε_{123}

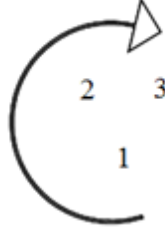


Figure 1: Demonstration of cyclic order

- $\varepsilon_{ijk} = -1$ when the indices i, j, k are different and form an odd permutation of (123), i.e. are in acyclic order. For example in Fig. 2, ε_{213}

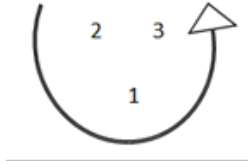


Figure 2: Demonstration of acyclic order

Free Indices and Dummy Indices

Free Indices

Free indices are the indices which occur only once in each tensor term. For example, i is the free index in the following tensor term:

$$v_{ij}w_j$$

In any tensorial expression, every term should have an equal number of free indices. For example, $v_{ij}w_j = c_j d_j$ is not a valid tensorial expression since the number of free indices is not equal in both terms.

Any free indices in a tensorial expression can be replaced by any other symbol as long as this symbol does not already occur in the expression. For example,

$$A_{ij}B_j = C_i D_j E_j \text{ is equivalent to } A_{kj}B_j = C_k D_j E_j$$

The number of free indices in an indicial equation gives the actual number of mathematical equations that will arise from it.

Dummy indices

Dummy indices are the indices that occur twice in the tensor terms. For example, j is the dummy index in $A_{ij}B_j$.

Any dummy index implies the summation of all components of that tensor term associated with each coordinate axis. Thus, when we write $A_i\delta_i$, we actually imply $\sum_{i=1}^3 A_i\delta_i$.

Any dummy index in a tensor term can be replaced by any other symbol as long as this symbol does not already occur in that term. For example, $A_{ijk}\delta_j\delta_k = A_{ipq}\delta_p\delta_q$

Note: The dummy indices can be renamed in each term separately, but free indices should be renamed for all terms in the tensor expression. For example, $A_{ij}B_j = C_iD_jE_j$ can be replaced by $A_{kp}B_p = C_kD_jE_j$.

Here, i is the free index which should be replaced by k in both terms but j is a dummy index so it can be replaced in only one term by p .

Summation convention in vector and tensor analysis

According to the Summation convention rule, if k is a dummy index which repeats itself in the expression then there should be a summation sign with it. Therefore, we can eliminate the implied summation sign and can write the expression in a more compact way. For example, using the Summation convention

$$\sum_k \sum_j \varepsilon_{ijk} \varepsilon_{ljk} \quad \text{can be simply written as} \quad \varepsilon_{ijk} \varepsilon_{ljk}$$

Relation between alternating unit tensor and Kronecker delta

When two indices are common between the two alternating unit tensors

$$\varepsilon_{ijk} \varepsilon_{ljk} = \sum_k \sum_j \varepsilon_{ijk} \varepsilon_{ljk} = 2\delta_{il} \quad (1)$$

When one index is common between the two alternating unit tensors

$$\varepsilon_{ijk} \varepsilon_{mnk} = \sum_k \varepsilon_{ijk} \varepsilon_{mnk} = \delta_{im} \delta_{jn} - \delta_{in} \delta_{jm} \quad (2)$$

A three by three determinant may be written in terms of the ε_{ijk}

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^3 \varepsilon_{ijk} a_{1i} a_{2j} a_{3k} \quad (3)$$

Mathematical operations on vectors

Addition of two vectors

$$\underline{u} + \underline{v} = u_i \underline{\delta}_i + v_i \underline{\delta}_i = \sum_{i=1}^3 (u_i + v_i) \underline{\delta}_i \quad (4)$$

In the same way, **subtraction** of vectors is done as

$$\underline{u} - \underline{v} = u_i \underline{\delta}_i - v_i \underline{\delta}_i = \sum_{i=1}^3 (u_i - v_i) \underline{\delta}_i \quad (5)$$

Dyadic Product of two vectors

The dyadic product is a mathematical operation on two vectors, which does not change the order of the resultant quantity. Since the order of the two vectors is one each, the order of tensor of the resultant is 2. Thus, the dyadic product of two vectors gives a second order tensor. To mathematically denote the dyadic product, we simply write the two vectors next to each other without any sign in between.

Example:

$$\underline{\delta}_i \frac{\partial}{\partial x_i} (v_j \underline{\delta}_j) \quad (6)$$

Here, $\underline{v} = v_j \underline{\delta}_j$ is velocity, i.e. a vector quantity and $\underline{\delta}_i \frac{\partial}{\partial x_i}$ is the gradient operator, also a vector quantity. Hence, the resultant $\frac{\partial v_j}{\partial x_i} \underline{\delta}_i \underline{\delta}_j$ (which physically represents the velocity gradient) is a second order tensor quantity.

Scalar product or dot product of two vectors

The dot product is a mathematical operation on two vectors, which reduces the order of tensor of the resultant quantity by two. Hence, dot product of two vectors has zero order, i.e. it is a scalar quantity. Mathematically, the dot product is defined as

$$\underline{v} \cdot \underline{w} = vw \cos(\phi_{vw})$$

where v and w denote the respective magnitudes of the two vectors, and ϕ_{vw} denotes the angle formed between the two vectors.

Vector product or cross product of two vectors

The cross product is a mathematical operation on two vectors, which reduces the order of tensor of the resultant quantity by one. Hence, cross product of two vectors has order unity, i.e. it is a vector quantity. Mathematically, the cross product is defined as

$$\underline{v} \times \underline{w} = v_i \underline{\delta}_i \times w_j \underline{\delta}_j = v_i w_j \underline{\delta}_i \times \underline{\delta}_j = vw \sin(\phi_{vw}) \underline{n}_{vw} \quad (7)$$

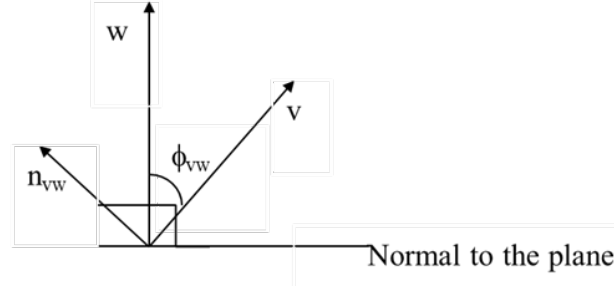


Figure 3: Cross product of vector v and w

Here in Fig.3, v and w denote the respective magnitudes of the two vectors, ϕ_{vw} denotes the angle between them, and \underline{n}_{vw} is a unit vector normal to \underline{v} and \underline{w} .