

Transport Model in Porous Media

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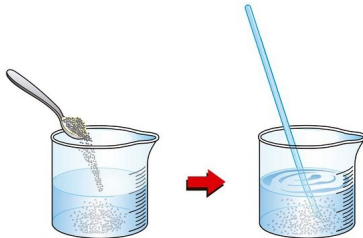
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Introduction

A brief discussion of the concepts of mixtures and solutions, which are generally well understood, may help to better understand the differences between one-phase and multicomponent systems.

For example, if salt (sodium chloride) is dissolved in water, at the beginning only one liquid phase is observed.



Introduction

The general procedure for constructing multiphase models is obtained by modifying slightly a three-step procedure:

- 1 A family of extensive properties is identified;
- 2 Each extensive property of the family is associated with one of the phases of the system; and
- 3 The balance conditions are applied to each extensive property of the family, using the particle velocity of the corresponding phase.

Introduction

Application of this strategy to the basic mathematical model of the multiphase system leads to the following system of differential equations:

$$\frac{\partial^\alpha}{\partial t} + \nabla \cdot (\underline{v}^\alpha \psi^\alpha) = \nabla \cdot \underline{\tau}^\alpha + \underline{g}^\alpha, \forall \alpha = 1, \dots, N \quad (1)$$

One must now define the constitutive equations and auxiliary (boundary and initial) conditions.

This complementary information about the systems plays a very important role since it is the means by which scientific and technological knowledge about a specific system is incorporated into the model.

Introduction

In single-fluid phase systems, it is assumed that the porous medium is saturated by the fluid; by this we mean that the fluid fills the pores completely, and therefore the volume of the pores equals the volume of the fluid that is contained in the porous medium.

The **fluid pressure** is also referred to as the pore pressure, especially in soil mechanics. The pressure in the pores pushes on the grain surfaces, exerting a force that tends to increase the pores' volume. In general, the grains move in response to changes in fluid pressure such that the porosity increases as the fluid pressure increases, and a decrease in pore fluid pressure results in a decrease in pore volume.

Transport Processes

The complementary information needed for the external supply g_i , since in a porous medium there may be exchange of solute with the solid matrix, which corresponds to chemical reactions and/or adsorption.

For this kind of solute transport, the random processes that contribute to the diffusive flux stem from two sources:

- 1 Molecular Brownian motion.
- 2 The random character of the pores channels.

So the diffusive flux $\underline{\tau}_i$ is the sum of two terms, the molecular diffusion and the mechanical dispersion, for which Fick's law adopts a special form.

Transport Processes

The basic framework in which it is necessary to incorporate the scientific and technological information available about the processes that occur in the transport system.

Three such processes will be distinguished:

- Advection
- diffusion
- mass generation

Advection

Whenever the fluid is in motion, advection occurs; that is, whenever the particle velocity is different from zero, $\underline{v} \neq 0$.

This phenomenon, or process, is due to the fact that the dissolved substance is carried by the fluid as it moves, just as a passenger is carried away by a bus.

The strength of the advective process is characterized by the fluid velocity, which in the transport models that are being considered is assumed to be a datum.

Thus, it is necessary to gather information about the particle velocity by suitable means.

Diffusion processes

The fact that a fluid is macroscopically at rest does not imply that the microscopic particles that constitute it are also at rest.

As a matter of fact, the microscopic particles that constitute a fluid (atoms, ions, or molecules) are in permanent agitation, and the solute particles that accompany them perform random walks known as Brownian motion.

Generally, the mass of solute particles that leave a fluid body due to such Brownian motion is not equal to the mass that enters it.

This imbalance produces a mass flux across the body boundary, and in macroscopic physics, phenomena of this kind are known as diffusion processes.

Diffusion processes

The diffusion process that is due to such a Brownian motion exclusively is known as molecular diffusion.

A simple experiment that evidences the occurrence of diffusion processes consists of depositing an ink drop in a pond containing water at rest. After awhile, the spot of ink spreads, getting larger and larger, and after a longer lapse, the ink concentration becomes distributed so evenly that it is imperceptible to the human eye.

Diffusion processes

When diffusion processes are very small in comparison with other processes that are taking place, satisfactory results can be obtained using models that ignore them. Such transport models are said to be non-diffusive.

A very simple model, albeit widely used, for molecular diffusion is *Fick's first law* it assumes that the vector field representing *the flux of solute mass*,

$$\underline{\tau}_s(\underline{x}, t) = \underline{\underline{D}} \cdot \nabla c \quad (2)$$

Here $\underline{\underline{D}}$ is a matrix, called the *tensor of molecular diffusion*, which is symmetric and non-negative.

Mass generation processes

The rate at which mass is generated is determined by the external supply, $g_S(\underline{x}, t)$.

When the external supply is identically zero, no mass is generated and each body of fluid conserves the mass of solute that it contains, except for the mass that comes through its boundary due to diffusion. In this case, the transport system is said to be conservative.

On the other hand, the solute mass is not conserved whenever the external supply of the solute is different from zero, $g_S(\underline{x}, t) \neq 0$, and such a transport system is said to be *non-conservative*.

Mass generation processes

Informally, one says that there is a mass source or a mass sink when $g_S(\underline{x}, t) > 0$ or $g_S(\underline{x}, t) < 0$, respectively.

Thus, it should be observed that the fact that $g_S(\underline{x}, t) \neq 0$ does not mean that such a principle is violated, since the mass conservation principle applies to isolated systems only.

Diffusion processes

To build the transport model we apply next assumptions:

We will introduce one-phase systems only, since we have assumed that at each point of the continuous system there is defined one and only one particle velocity.

In this section Flow of fluids in a porous medium; that is fluids that are restricted to move in the voids of a porous material.

The basic **mathematical model** of fluid flow in a porous medium will be developed. Generally, the final goal of this kind of model is to predict the flow of the fluid (that is, the fluid velocity).

A **porous medium**, is a solid material that contains voids in its interior that are interconnected such that the flow of fluid through them is possible. The solid material that forms the porous medium is referred to as the **solid matrix**.

Introduction

A porous medium is a solid material that contains voids in its interior that are interconnected such that the flow of fluid through them is possible.

The solid material that forms the porous medium is referred to as the solid matrix.

The voids are the pores, and the volume fraction of the physical space that is occupied by the pores is the porosity.

Introduction

In single-fluid phase systems, it is assumed that the porous medium is saturated by the fluid;

The fluid fills the pores completely.

The volume of the pores equals the volume of the fluid that is contained in the porous medium.

If the fluid contains a solute, the mass of solute per unit fluid volume is again referred to as the concentration.

The fluid motion takes place in the pores, and the fluid particle velocity is $\underline{v}_f(\underline{x}, t)$

Introduction

The mass $M_{Si}(t)$ of solute i contained in a body of fluid is also an extensive property, and the intensive property associated with the solute mass is equal to the porosity $\phi(\underline{x}, t)$ multiplied by $c_i(\underline{x}, t)$ the concentration of solute i .

$$M_{Si}(t) = \int_{\Omega(t)} \phi(\underline{x}, t) c_i(\underline{x}, t) d\underline{x} \quad (3)$$

where $i = 1, \dots, m$ is the number of solutes contained in the fluid.

Introduction

The global balance equation is

$$\frac{dM_{Si}}{dt}(t) = \int_{\Omega(t)} g_i(\underline{x}, t) \, d\underline{x} + \int_{\Omega(t)} \underline{\tau}_i(\underline{x}, t) \cdot \underline{n}(\underline{x}, t) \, d\underline{x} \quad (4)$$

The external supply of the solute under consideration, $g_i(\underline{x}, t)$, can be different from zero for several reasons; for example, it may be attributable to radioactive decay.

The expression $\underline{\tau}_i(\underline{x}, t) \cdot \underline{n}(\underline{x}, t)$ represents the mass of solute per unit area, per unit time, that enters the body of fluid. In the case of a free fluid the flux of solute mass, $\underline{\tau}_i(\underline{x}, t)$, occurs mainly due to molecular diffusion.

Introduction

The local balance equation for the multicomponent transport of different solutes by a fluid contained in a porous medium is the system of differential equations:

$$\frac{\partial \phi c_i}{\partial t} + \nabla \cdot (\phi c_i \underline{v}_f) = \nabla \cdot \tau_i + g_i \quad (5)$$

the fluid motion in the porous medium needs to be known.

In practice, one frequently derives these functions by modeling the flow of the fluid before modeling the solute transport.

In order to have a complete model for the transport of a solute, we need to be supplemented with scientific and technical information about \underline{v}_f , the particle velocity, τ_i , the solute-mass flux, and g_i , the external supply of solute mass.

Introduction

Transport processes:

- Advection
- Mass generation (non-conservative processes)
- dispersion-diffusion

Introduction

Advection: occurs whenever the fluid velocity is different from zero and its intensity depends on the magnitude of \underline{v} .

This phenomenon, or process, is due to the fact that the dissolved substance is carried by the fluid particles as they move.

We observe that in the case of transport by a fluid in a porous medium, two kinds of velocities were defined:

- The velocity of fluid particles, \underline{v}
- The Darcy velocity, \underline{u}

these two velocities are related by $\underline{u} = \phi \underline{v}$.

Introduction

Mass generation (non-conservative processes)

Mass generation of the solutes may occur by chemical reactions, radioactive decay, and adsorption of the solute by the solid matrix.

- First-order irreversible processes
 - * the mass source
 - * first-order chemical reactions and radioactive decay
- Adsorption

Introduction

First-order irreversible processes

A convenient notation to express the mass source in the case when the fluid is contained in a porous medium is

$$g_S = \phi \hat{g}_S \quad (6)$$

g_S represents the solute mass source per unit time, per unit volume of the physical space occupied by the solid-fluid system,

\hat{g}_S is the mass source per unit time, per unit volume of the fluid.

Then, for first-order chemical reactions and radioactive decay, \hat{g}_S is

$$g_S = \phi \hat{g}_S = -\lambda \phi c \quad (7)$$

Introduction

Adsorption

Adsorption is a well-known phenomenon identified with solute transport in a porous medium.

Adsorption is a phenomenon that occurs due to the presence of the solid matrix when the transport of solutes takes place in a porous medium.

This process is a type of chemical reaction in which the solute interacts with the solid phase of the porous medium.

Introduction

A precise and rigorous treatment of adsorption, requires approaching the fluid-solid system as a system made up of two phases and two components:

- The phases are the solid matrix and the fluid contained in it.
- The components of the porous medium are the solute dissolved in the fluid and the solute contained on the solid substance that constitutes the solid matrix.

Thus, we have to build a model in which two components are contained by the solid phase while one is contained by the fluid.

Introduction

The following notation will be used for building such a model:

g_S^f is the solute mass source that goes from the solid phase to the fluid phase

g_f^S is the solute mass source that goes from the fluid phase to the solid phase

ρ_S is the density of the solid phase (mass of solid over volume of solid)

$\rho_b = (1 - \phi)\rho_S$, is the bulk density of the solid phase (mass of solid over total volume of porous medium)

ϖ is the mass fraction of the solute in the solid phase (mass of solute over mass of solid).

Introduction

Dispersion-diffusion

Diffusion processes are also modeled by means of Fick's law; however, for this kind of application it is usually written in the form

$$\underline{\tau}_S = \phi \underline{\underline{D}} \nabla c \quad (8)$$

two different kinds of phenomena coexist in diffusion processes that occur in a fluid contained in a porous medium:

- *Molecular diffusion*, which is due to Brownian motion occurring at the microscopic level
- *Mechanical dispersion*, which is due to the tortuous fluid flow attributable to the randomness of the solid-matrix structure.

Introduction

Each of these phenomena contributes to the overall dispersion-diffusion process where they have an additive effect.

The dispersion tensor $\underline{\underline{D}}$ is expressed as the sum of the tensor $\underline{\underline{D}}^m$ of molecular diffusion plus the tensor $\underline{\underline{D}}^M$ of mechanical dispersion

$$\underline{\underline{D}} = \underline{\underline{D}}^m + \underline{\underline{D}}^M \quad (9)$$

Mechanical dispersion does not occur when the fluid is at rest, but when the fluid is in motion the effect of mechanical dispersion is usually more significant than that of molecular diffusion.

Conceptual Model

The following assumptions are usually adopted for models of transport of solutes by a fluid:

- The fluid motion is known beforehand; in particular, the fluid velocity is provided as a datum through the flow model.
- The fluid is located in the pores of a porous medium.
- The porous medium is saturated; that is, that the fluid fills completely the pores.
- The fluid does not fill the physical space since part of it is occupied by the solid matrix.

Mathematical Model

The mass of solute, $M_S(t)$, contained in a body of a porous system, which is made up of the solid matrix and the fluid, is given by the integral

$$M_S(t) = \int_{\Omega(t)} \phi(\underline{x}, t) c(\underline{x}, t) d\underline{x} \quad (10)$$

Here $c(\underline{x}, t)$ is the concentration of the solute, that is, the mass of solute per unit volume of the fluid, and $\phi(\underline{x}, t)$ is the porosity.

Mathematical Model

On the other hand, the global balance equation is

$$\frac{d}{dt} M_S(t) = \int_{\Omega(t)} g_S(\underline{x}, t) \, d\underline{x} + \int_{\partial\Omega(t)} \underline{\tau}_S(\underline{x}, t) \cdot \underline{n}(\underline{x}, t) \, d\underline{x} \quad (11)$$

where

$g_S(\underline{x}, t)$ represents the solute mass sources

$\underline{\tau}_S(\underline{x}, t)$ is the solute mass flux, due to the diffusion-dispersion processes.

Mathematical Model

Now applying the axiomatic formulation of continuous models, the local balance equation is

$$\frac{\partial}{\partial t}(\phi c) + \nabla \cdot (\phi c \underline{v}) = g_S + \nabla \cdot \underline{\tau}_S \quad (12)$$

this equation must be fulfilled at every point occupied by the solid-matrix-fluid system.

Mathematical Model

Exercise:

To write the "local balance equation" (1 minute)

$$\text{if } \psi = \phi c, \text{ with } \phi = R(\underline{x}, t)$$

$$\phi \underline{v} = \underline{u}$$

$$g = -rc + f, \text{ with } r = \text{constant}$$

$$\tau = \underline{\underline{D}} \cdot \nabla c$$

Mathematical Model

Therefore, the basic mathematical model for the transport of a solute by a fluid contained in a porous medium is:

$$R \frac{\partial c}{\partial t} - \nabla \cdot (\underline{\underline{D}} \cdot \nabla c) + \nabla \cdot (\underline{u} c) + rc = f, \quad \forall \underline{x} \in \Omega, t \geq t_0 \quad (13)$$

$$c = c^0, \quad \forall \underline{x} \in \Omega \text{ y } t = t_0 \quad (14)$$

$$c = c_\partial, \quad \forall \underline{x} \in \partial_D \Omega \text{ y } t > t_0 \quad (15)$$

$$-\underline{n} \cdot (\underline{\underline{D}} \cdot \nabla c) = g_\partial, \quad \forall \underline{x} \in \partial_N \Omega \text{ y } t > t_0 \quad (16)$$

This is a general parabolic differential equation of second order.

Here, c is the concentration, $\underline{\underline{D}}$ is the dispersion-diffusion tensor, \underline{u} is the Darcy velocity, r is the reaction term.

Numerical Model

Let superscript n denote a quantity at time t_n , where n is an integer counting time levels. So, $c^n \equiv c(\underline{x}, t_n)$ means c at time level n .

$$R \frac{\partial c^n}{\partial t} - \nabla \cdot (\underline{\underline{D}}^n \cdot \nabla c^n) + \nabla \cdot (\underline{u}^n c^n) + r^n c^n = f^n \quad (17)$$

For simplicity and stability reasons, the time-derivative can be approximated by a simple backward finite difference.

$$\frac{\partial c^n}{\partial t} \approx \frac{c^n - c^{n-1}}{\Delta t_n} \quad (18)$$

where

$$\Delta t_n \equiv t_n - t_{n-1}$$

with $n = 1, \dots, N$ is the time discretization parameter.

Numerical Model

Inserting (18) in (17) yields

$$R^n \frac{c_i^n - c^{n-1}}{\Delta t_n} - \nabla \cdot (\underline{\underline{D}}^n \cdot \nabla c^n) + \nabla \cdot (\underline{u}^n c^n) + r^n c^n = f^n \quad (19)$$

Exercise:

Reordering the equation (19) such that the terms with the unknown c^n appears on the left-hand side and the right-hand side contains the computed terms at the previous time level c^{n-1} only

$$\left(\frac{R^n}{\Delta t_n} + r^n \right) c^n - \nabla \cdot (\underline{\underline{D}}^n \cdot \nabla c^n - \underline{u}^n c^n) = \frac{R^n}{\Delta t_n} c^{n-1} + f^n \quad (20)$$

Given $c^0 = c_0$, we can solve for c^1 , c^2 , c^3 , and so on.

Numerical Model

if we multiply (20) by the test function w and integrate over Ω :

$$\begin{aligned} & \int_{\Omega} \left(\frac{R^n}{\Delta t_n} + r^n \right) c^n w d\underline{x} - \int_{\Omega} \nabla \cdot (\underline{\underline{D}}^n \cdot \nabla c^n - \underline{u}^n c^n) w d\underline{x} \\ &= \int_{\Omega} \left(\frac{R^n}{\Delta t_n} c^{n-1} + f^n \right) w d\underline{x} \end{aligned} \quad (21)$$

where

$$\begin{aligned} c &\in W = \{c \in H^1(\Omega) \mid c = c_{\partial}, \quad \forall \underline{x} \in \partial_D \Omega\} \\ w &\in \hat{W} = \{w \in H^1(\Omega) \mid w = 0, \quad \forall \underline{x} \in \partial_D \Omega\} \end{aligned}$$

Numerical Model

Homework:

Applying integration by parts to the integrand with second-order derivatives and after applying the boundary condition (16):

$$\begin{aligned}
 & \int_{\Omega} \left(\frac{R^n}{\Delta t_n} + r^n \right) c^n w \, d\underline{x} + \int_{\Omega} \nabla w \cdot (\underline{\underline{D}}^n \cdot \nabla c^n - \underline{u}^n c^n) \, d\underline{x} \\
 & + \int_{\partial\Omega_N} w \, c^n \underline{u}^n \cdot \underline{n} \, d\underline{x} \\
 & = \int_{\Omega} \left(\frac{R^n}{\Delta t_n} c^{n-1} + f^n \right) w \, d\underline{x} - \int_{\partial\Omega_N} w \, g_{\partial} \, d\underline{x} \quad (22)
 \end{aligned}$$

Remember that $w \in \hat{W} = \{w \in H^1(\Omega) \mid w = 0, \quad \forall \underline{x} \in \partial_D \Omega\}$.

Numerical Model

We need to transform the continuous variational problem (22) to a discrete variational problem.

Find $c_h^n \in W$ such that $a(c_h^n, w_h) = L_n(w_h), \forall w_h \in \hat{W}_h$, for $n = 1, 2, \dots, N$, where

$$\begin{aligned} a(c_h^n, w_h) &= \int_{\Omega} \left(\frac{R^n}{\Delta t_n} + r^n \right) c_h^n w_h + \nabla w_h \cdot (\underline{\underline{D}}^n \cdot \nabla c_h^n - \underline{u}^n c_h^n) d\underline{x} \\ &+ \int_{\partial_N \Omega} c_h^n w_h \underline{u}^n \cdot \underline{n} d\underline{x} \end{aligned} \quad (23)$$

$$L(w_h) = \int_{\Omega} \left(\frac{R^n}{\Delta t_n} c_h^{n-1} + f^n \right) w_h d\underline{x} - \int_{\partial_N \Omega} w_h g_{\partial} d\underline{x} \quad (24)$$

FEniCS script with Python

```
from fenics import *
from mshr import *
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

# Define 2D geometry and generate mesh
domain = Rectangle(Point(xmin,ymin),Point(xmax,ymax))
mesh = generate_mesh(domain, 30)

# Define function space
fs_order = 1 # function space order
V = FunctionSpace(mesh, 'Lagrange', fs_order)

n = FacetNormal(mesh)
PecletGlobal=100
```

Listing 1: Python script

FEniCS script with Python

```
# Data of the Problem:

R=1 # Adsorption term
u_in=0.0223/day # Injection velocity [m/s]
u_x=0 # Darcy velocity in the x-direction [m/s]
u_y=u_in # Darcy velocity in the y-direction [m/s]
alfa_L=1/PecletGlobal#Longitudinal dispersion coeff[m]
alfa_T=0 # Transversal dispersion coefficient [m]
D_xx= alfa_L*u_x # [m2/s]
D_xy=0 # [m2/s]
D_yx=D_xy # [m2/s]
D_yy= alfa_L*u_y # [m2/s]
q_c=0 # Source term
c0= 1326.2 # Initial concentration [ppm]
c_in=c0/100 # [ppm]
# Hydrodynamic dispersion tensor
D = as_matrix(((D_xx, D_xy), (D_yx, D_yy)))
u = as_vector([u_x, u_y]) # Vector velocity
```

Listing 2: Python script

FEniCS script with Python

```
# Boundary Conditions
boundary_parts = FacetFunction("size_t", mesh)

#Boundary condition at the bottom
class BottomBoundary(SubDomain):
    def inside(self, x, on_boundary):
        tol = 1E-14 # tolerance for coordinate comparisons
        return on_boundary and abs(x[1] - ymin) < tol

Gamma_1 = BottomBoundary()
Gamma_1.mark(boundary_parts, 1)

#If Dirichlet condition
c_B = Constant(c_in)
bc1=DirichletBC(V, c_B, boundary_parts, 1)
```

Listing 3: Python script

FEniCS script with Python

```
# Boundary condition at the top
class TopBoundary(SubDomain):
    def inside(self, x, on_boundary):
        tol = 1E-14 # tolerance for coordinate comparisons
        return on_boundary and abs(x[1] - ymax) < tol

Gamma_3 = TopBoundary()
Gamma_3.mark(boundary_parts, 3)

#If Dirichlet condition
c_T = Expression('1 + 2*x[1]*x[1]', degree=fs_order)
bc3=DirichletBC(V, c_T, boundary_parts, 3)

#If any Dirichlet condition
bcs = [bc1]
```

Listing 4: Python script

FEniCS script with Python

```
#Initial condition
c_0 = Expression('c0 + t', c0=c0, t=t_0, degree=fs_order)
c_1 = project(c_0, V)

# Define Trial and Test functions
c = TrialFunction(V)
w = TestFunction(V)

# Variational forms and problem
a = R*c*w*dx + dt*inner(nabla_grad(w), dot(D, nabla_grad(c))-
    u*c)*dx + dt*u_y*c*w*ds(3)
L = (R*c_1 + dt*q_c)*w*dx #- dt*g_in*w*ds(1)

# the unknown at a new time level
c = Function(V)
```

Listing 5: Python script

FEniCS script with Python

```
# Time
t_0=0 # Initial time [s]
t_N=400000 # End time [s]
dt = 2500 # Time step
NT=int((t_N-t_0)/dt) # Number of time steps

while t < t_N:
    b = assemble(L, tensor=b)
    c_0.t = t
    for bc in bcs:
        bc.apply(A, b) #if Dirichlet conditions
    solve(A, c.vector(), b)
    t += dt
    i=i+1
    c_1.assign(c)
    c_e = interpolate(c_0, V)
    ch = project(c)
```

Listing 6: Python script

Validation Problem

- Here goes the validation Problem section...

Case Study

- Here goes the Case Study section...

Final Remarks

- Final Remarks

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Thank you

Questions or Comments