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| ESEIAAT - UPC |
| Study for the computational resolution of conservation equations of mass, momentum and energy. Possible application to different aeronautical and industrial engineering problems: Case 1B |
| Report |
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| **[Seleccione la fecha]** |

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# Introduction

# State of the art

The laws governing the processes of heat transfer and fluid flow are usually expressed in terms of differential equations. Some of these equations are the momentum equation, the energy equation and the mass conservation equation, among others. However, these expressions usually don’t have an analytical solution except for some simple cases. To solve complex problems it is necessary to use numerical methods.

## Conservation equations

The three most important conservation equations are the mass conservation equation, the momentum conservation equation and the energy conservation equation:

For incompressible flows with no viscous dissipation, the energy conservation equation can be written as:

All these equations can be seen as a particular case of the generic convection-diffusion equation:

Where is the density, the velocity, the diffusion coefficient, the source term, and the general variable that is going to be studied.

|  |  |  |  |
| --- | --- | --- | --- |
| Equation | φ | Γ | Sφ |
| Mass conservation | 1 | 0 | 0 |
| Momentum |  | μ |  |
| Energy (for a semi perfect gas) | u | λ/cv |  |

Table 1: Particular cases of the convection-diffusion equation

## Numerical methods

Numerical methods are based in dividing the domain that is going to be studied in different pieces. Instead of calculating the unknowns in the whole domain, they are studied in the finite number of points defined by these pieces, the grid points. This process is called discretization.

Once the domain is discretized, it is also necessary to discretize the equations. The relations between the grid points have to be established. It is assumed that the value of a grid point only influences the distribution of in its immediate neighbours. For this reason, as the number of grid points becomes larger, the numerical solution approaches the real solution of the problem.

There are different methods of discretizing the equations, but the most common ones are exposed in the following lines.

### Finite difference method

The finite difference method (FDM) is based in the Taylor-series expansion. It is used to approximate the derivatives in the differential equation. Taking the three successive points represented in Figure 1, the approximation of the values in the left point (west) and in the right point (east) is easily calculated with Taylor series:

Using a second order approximation and combining both expressions, it can be easily obtained:

These expressions are substituted in the differential equation to obtain the finite-differential equation. This approach is very simple, but it is not used in complex geometries. It also does not enforce the conservation, as it is simply a mathematical approach, which may lead to some problems.

P

W

E

Figure 1: Three successive grid points

### Finite volume method

The finite-volume method (FVM) is more used than the FDM. It consists in dividing the domain in different control volumes, so that each control volume surrounds one grid point. Then, the differential equation is integrated over each control volume, ensuring that each of them satisfy the conservation.

P

W

E

S

Figure 2: Control volume (2D)

## Time integration

Time is a one-way variable, which means that the variables only depend on the values of the previous instant of time, and do not depend on the values of the next instant of time. Taking this property into account, to obtain the results of an unsteady problem, the method is to discretize the time and calculate the values for each time step. When the values of one time step are obtained, the calculation moves on to the next time step.

Time integration can be done using different methods. The ones that are widely used are:

* Implicit method
* Crank-Nicholson
* Explicit method

## Values on the faces

# Four materials

The four materials problem is a two-dimensional transient conduction problem. It consists in a long rod composed of four different materials with different properties. The general scheme of the problem is represented in Figure 1:

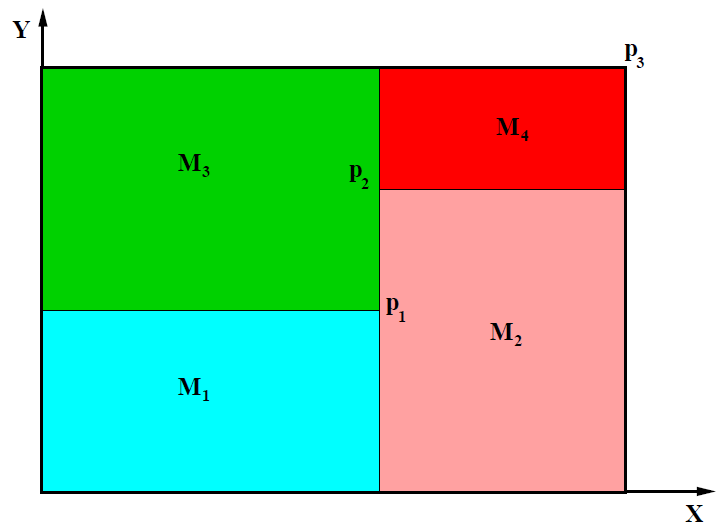


Figure 3: General scheme of the four materials problem

|  |  |  |
| --- | --- | --- |
|  | x [m] | y [m] |
| p1 | 0.50 | 0.40 |
| p2 | 0.50 | 0.70 |
| p3 | 1.10 | 0.80 |

Table 2: Problem coordinates

|  |  |  |  |
| --- | --- | --- | --- |
|  | ρ [kg/m3] | cP [J/kgK] | λ [W/mK] |
| M1 | 1500.00 | 750.00 | 170.00 |
| M2 | 1600.00 | 770.00 | 140.00 |
| M3 | 1900.00 | 810.00 | 200.00 |
| M4 | 2500.00 | 930.00 | 140.00 |

Table 3: Physical properties of the materials

|  |  |
| --- | --- |
| Cavity wall | Boundary condition |
| Bottom | Isotherm at |
| Top | Uniform length |
| Left | In contact with a fluid at and heat transfer coefficient |
| Right | Uniform temperature (where is the time in seconds) |

Table 4: Boundary conditions

The initial temperature field is .

## Conduction equation

The conduction heat transfer is described by Equation 1:

Equation 1: Conduction equation

Where is the density, the temperature, the conductivity of the material, the specific heat of the material and the inner heat of the material (source term).

## Discretization

The domain is discretized using the node centred distribution, to avoid having conflictive control volumes between the different materials. Since it is a transitory problem, it is necessary to discretize in space and time. The method used to discretize the equation is the finite volume method.

### Space discretization

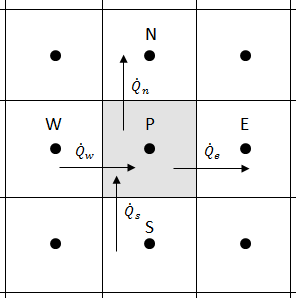


Figure 4: Heat fluxes through the faces of a control volume

The heat fluxes through the walls represented in Figure 2 are integrated:

Equation 2: Discretized heat fluxes through the walls

Where is the temperature at the given node, the distance between two nodes, and the conductivity at the given face.

However, since there are different materials there are faces in which the conductivity can have two values: one on the left side of the face and the other one on the right side of the face. This problem is solved with the harmonic mean. It can be calculated with the heat fluxes through the wall:

Equation 3: Harmonic mean

The inner heat of the material can be discretized as:

Equation 4: Discretized inner heat flux (source term)

### Time discretization

The time discretization is done using the First law of thermodynamics:

Where is the internal energy of the control volume.

Assuming and , the First law of thermodynamics is integrated over time. Taking as the previous instant of time and the instant of time that is going to be calculated:

Taking the first term of the equation:

And the second term:

Finally, the discretized equation is:

Equation 5: Discretized conduction equation

So that the discretized coefficients are:

Equation 6: Discretization coefficients for the four materials problem

### Boundary conditions

The outer walls of the rod have special conditions, so each of them has to be studied in order to determine the coefficients of the boundary nodes.

In the left wall (), there is convection, so the coefficients have to be recalculated:

The only coefficients that change are:

Equation 7: Discretization coefficients of the left wall

In the top wall () there is a constant heat flux, so that the new equation is:

The new coefficients are:

Equation 8: Discretization coefficients of the top wall

In the right wall (), the temperature is given, and it changes over time. The conduction equation becomes:

The coefficients are very similar to those of the general case. The only differences are:

Equation 9: Discretization coefficients of the right wall

Finally, in the bottom () the temperature is also given, but it is constant. The approach is very similar to that of the right wall.

So that the coefficients are:

Equation 10: Discretization coefficients of the bottom wall

## Algorithm

YES

YES

Input data:

Previous calculations:

Initial temperature map:

Calculation of the next time step:

Evaluation of the constant coefficients:

Solve the set of equations:

Final calculations and print results

END

?

New time step?

NO

NO

Evaluation of the non-constant coefficients:

## Results

# Smith-Hutton problem

The following problem is a two-dimensional steady convection-diffusion problem, represented in Figure 2:

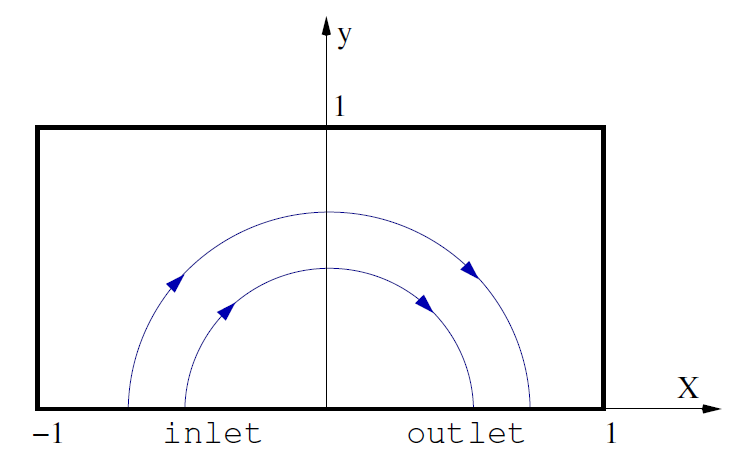


Figure 5: General scheme of the Smith-Hutton problem

The velocity field is given by:

Equation 11: Prescribed velocity

And the boundary conditions for the variable are:

Equation 12: Boundary conditions of the Smith-Hutton problem

Where .

## General convection-diffusion equation

The mathematical formulation needed to solve this problem is the convection diffusion-equation:

Equation 13: Generic convection-diffusion equation

## Discretization

It is necessary to discretize Equation 2 in space and time. The control volume used to discretize the problem is specified in Figure 1:

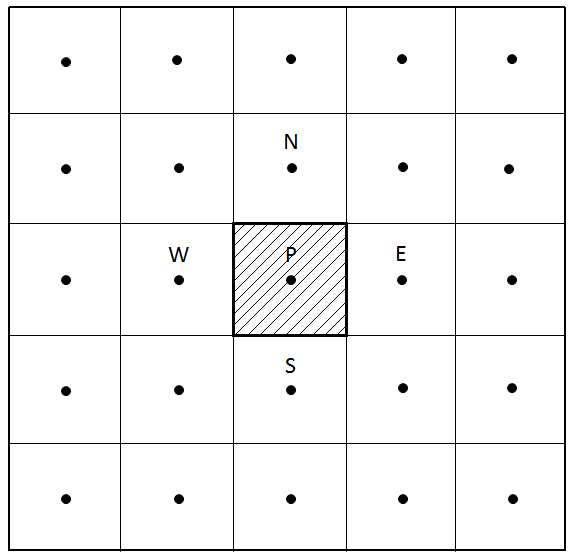


Figure 6: Control volumen (2D)

To do so, it is easier to start with the discretization of the mass equation:

Equation 14: Mass conservation equation

The first step is to integrate Equation 3 over time and space. Taking only the first term of the equation:

Using the Divergence Theorem, the second term of the equation transforms into a surface integral:

In the second term, to integrate over time an implicit scheme is used. The final discretized mass equation is:

Equation 15: Discretized mass equation (2D)

The discretization of the convection-diffusion equation is very similar to that of the mass equation. Integrating over the volume the transport term of Equation 2 and applying the Divergence Theorem:

The same procedure is used for the diffusion term:

Where:

To simplify the source term, it is linearized:

So that the resulting equation is:

Multiplying by the discretized mass equation (Equation 4) and subtracting the result in this equation, the discretized convection-diffusion equation is obtained:

To simplify the problem, a new variable is introduced to the problem: the total flux. But this variable is split in the two dimensions of the problem, the flux in the x-direction and the flux in the y-direction.

Equation 16: Total (convection plus diffusion) fluxes

Introducing the expressions of the total flux, the discretized convection diffusion equation becomes:

Equation 17: Final discretization of the convection diffusion equation

Where the flow rates are:

However, it is necessary to know how the fluxes are going to be evaluated. In order to use adimensional numbers, a new variable is defined:

Where is the Peclet number and is the distance between the point that is going to be studied *i*, and the point next to it, *i+1*. The value of φ and the value of the gradient are a combination of the and , so that can be expressed as:

The coefficients and are dimensionless and depend on the Peclet number. However, since B is a combination of A and the Peclet number, and both coefficients are symmetric, it can be deduced that:

Equation 18: Dimensionless coefficients A and B

Where is an operator that denotes the greater of A and B.

Combining Equation 6 and Equation 7, the following formulation is obtained:

Where

Equation 19: Discretization coefficients of the Smith-Hutton problem

And the Peclet numbers are:

The only operation that should be defined is the value of the coefficient . This value depends on the integration scheme that is going to be used. Some of its values are in Table 2:

|  |  |
| --- | --- |
| Scheme | Formula for |
| Central difference (CDS) |  |
| Upwind (UDS) |  |
| Hybrid (HDS) |  |
| Power law (PLDS) |  |
| Exponential (EDS) |  |

Table 5: Function for different schemes1

For a better explanation of the different schemes used, search PATANKAR.

## Boundary conditions

To apply the boundary conditions to the problem, some modifications on the coefficients defined by Equation 10 have to be done. The easiest one is for the points in the left, top and right sides of the domain, in which the value of is defined.

Equation 20: Discretization coefficients for the boundary points

In the bottom it is necessary to distinguish between the inlet and the outlet. A similar approach to that of the left, top and right side is used to determine the coefficients of the points in the inlet:

Equation 21: Discretization coefficients for the inlet

However, the most difficult point is that of the outlet. The only condition is that the derivative of in the vertical direction is equal to zero. Following this reasoning, the following coefficients are obtained:

Equation 22: Discretization coefficients for the outlet

## Results