HAMT - Tool for simulation of Heat And Mass Transfer

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1 Numerics

1.1 Finite Difference Method - FDM

First order Discritization.

$$f_f' = \frac{f_{i+1} - f_i}{\Delta x} \tag{1.1}$$

$$f_b' = \frac{f_i - f_{i-1}}{\Delta x} \tag{1.2}$$

$$f'_{c} = \frac{1}{2} \left(f'_{f} + f'_{b} \right) = \frac{1}{2} \left(\frac{f_{i+1} - f_{i}}{\Delta x} + \frac{f_{i} - f_{i-1}}{\Delta x} \right) = \frac{f_{i+1} - f_{i-1}}{2 \Delta x}$$
 (1.3)

second order

$$f'' = \frac{f_f' - f_b'}{\Delta x} = \frac{f_{i+1} - f_i}{\Delta x^2} - \frac{f_i - f_{i-1}}{\Delta x^2} = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$
(1.4)

Assuming the differentials $a \frac{\partial f}{\partial x}$ and $a \frac{\partial^2 f}{\partial x^2}$ where a is not constant.

$$a f_c' = \frac{1}{2} \left(\frac{a_{i+1}(f_{i+1} - f_i)}{\Delta x} + \frac{a_{i-1}(f_i - f_{i-1})}{\Delta x} \right) = \frac{a_{i+1}f_{i+1} + (a_{i-1} - a_{i+1})f_i - a_{i-1}f_{i-1}}{2\Delta x}$$
 (1.5)

$$a f'' = a_{i+1} \frac{f_{i+1} - f_i}{\Delta x^2} - a_{i-1} \frac{f_i - f_{i-1}}{\Delta x^2} = \frac{a_{i+1} f_{i+1} - (a_{i+1} + a_{i-1}) f_i + a_{i-1} f_{i-1}}{\Delta x^2}$$
(1.6)

1.1.1 Dirichlet Boundary Conditions

$$f|_i = f_0 \tag{1.7}$$

1.1.2 Neumann Boundary Conditions

$$\left. \frac{\partial f}{\partial x} \right|_{x=i} = c \tag{1.8}$$

$$\frac{f_i - f_i - i}{\Delta x} = c \tag{1.9}$$

$$f_i - f_{i-i} = \Delta x c \tag{1.10}$$

2 Heat Transfer

The base equation for the heat transfer is the balance equation of the form

$$\frac{\partial \rho}{\partial t} + \nabla \vec{j} = f(\vec{r}, t) \tag{2.1}$$

where ρ is the density of the quantity in question, \vec{j} is the flux, \vec{r} is the position vector and t is time. For heat transfer problem we define ρ as the volumetric heat density q which is defined as

$$q = \frac{Q}{V} = c \rho T \tag{2.2}$$

 $ec{j}$ is equivalent to the heat flux $ec{q}$

$$\vec{\dot{q}} = -\lambda \, \nabla T \tag{2.3}$$

and the source $f(\vec{r},t)$ is the volumetrix heat source $\dot{q}_v(\vec{r},t)$. Inserting 2.2 and 2.3 in 2.1 leads to the heat transfer equation

$$\frac{\partial(c\,\rho\,T)}{\partial t} + \nabla(-\lambda\,\nabla T) = \dot{q}_v(\vec{r},t) \tag{2.4}$$

where the quantities are defined as seen in table 2.1.

Table 2.1: Heat Transfer - parameters

Quantitiy	Description	Unit
c	Specific heat capacity	$ m Jkg^{-1}K^{-1}$
ho	Density	${\rm kgm^{-3}}$
T	Temperature	K
λ	Thermal conductivity	${ m W}{ m m}^{-1}{ m K}^{-1}$
\dot{q}_v	Volumetric heat source	$ m Wm^{-3}$

2.1 Homogeneous Heat Transfer Equation

Aussuming...

$$\lambda \, \Delta T = 0 \tag{2.5}$$

2.2 FDM - Homogeneous Equidistant 2D

2.2.1 Boundary Conditions

For all boundary condition is present the dirichlet boundary conditions always orride other boudnary conditions on contact nodes. If two cells with different dirichlet boundary conditions touch, a arichmetical mean is taken.

Corner Boundary Conditions

Examples buttom left corner

$$T_{i+1,j} - T_{i,j} = \Delta x_1 c_1 \tag{2.6}$$

$$T_{i,j+1} - T_{i,j} = \Delta x_2 c_2 \tag{2.7}$$

By adding the two functions one gets

$$T_{i+1,j} + T_{i,j+1} - 2T_{i,j} = \Delta x_1 c_1 + \Delta x_2 c_2. \tag{2.8}$$

Radiation Boundary Conditions

$$\vec{q}_r = \epsilon \, \sigma \, T^4 \, \vec{n} \tag{2.9}$$

Using the Taylor series

$$T f(x; a) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!} (x - a)^n$$
 (2.10)

we get the linearized equation for the heat flux due to radiation

$$T \dot{q}_r(T; T_0) = (4 \epsilon \sigma T_0^3) T - 3 \epsilon \sigma T_0^4. \tag{2.11}$$

Using eqation (2.3)

$$-\lambda \frac{\partial T}{\partial x} = T \,\dot{q}_r(T; T_0) \tag{2.12}$$

leads to the discitized, linear equation

$$(1 + 4kT_0^3)T_i - T_{i-1} = 3kT_0^4$$
(2.13)

where

$$k = \frac{\epsilon \, \sigma \, \Delta x}{\lambda} \tag{2.14}$$

Table 2.2: Radiation Boundary Condition - parameters

Quantitiy	Description	Unit
ϵ	Emissivity factor	_
σ	Stefan-Boltzmann constant	$ m W m^{-2} K^{-4}$
Δx	Spatial step	m

2.2.2 Cartesian Coordinates

The homogeneous heat equation in cartesian coordinates is expressed as

$$\lambda \frac{\partial^2 T}{\partial x^2} + \lambda \frac{\partial^2 T}{\partial y^2} + \lambda \frac{\partial^2 T}{\partial z^2} = 0 \tag{2.15}$$

By assuming only the x and y directions equation (2.15) reduces to

$$\lambda \frac{\partial^2 T}{\partial x^2} + \lambda \frac{\partial^2 T}{\partial y^2} = 0. \tag{2.16}$$

Using equation (1.6) equation (2.16) can be discritizised as

$$\lambda_{i+1,j}T_{i+1,j} + \lambda_{i,j+1}T_{i,j+1} - \lambda_{tot}T_{i,j} + \lambda_{i-1,j}T_{i-1,j} + \lambda_{i,j-1}T_{i,j-1} = 0$$
(2.17)

where

$$\lambda_{tot} = \lambda_{i+1,j} + \lambda_{i-1,j} + \lambda_{i,j+1} + \lambda_{i,j-1}. \tag{2.18}$$

In case any of the λ paramters is to be taken on a boundary between two segments, a mean between to is to take. The correctness of this assumptions can be proven by setting up 4 equations around a center node using Fourrier's law. For $\lambda = const$ the equation reduces to

$$T_{i+1,j} + T_{i,j+1} - 4T_{i,j} + T_{i-1,j} + T_{i,j-1} = 0 (2.19)$$

2.2.3 Cylinder Coordinates

while in cylinder coordinates as

$$\lambda \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \lambda \frac{1}{r^2} \frac{\partial^2 T}{\partial \phi^2} + \lambda \frac{\partial^2 T}{\partial z^2} = 0. \tag{2.20}$$

2.2.4 Verification

Heat codnuctivity trhough a layerd wall

$$\dot{q} = \left(\sum_{i=1}^{N} \frac{\Delta x_i}{\lambda_i}\right)^{-1} \Delta T \tag{2.21}$$