DIRECTION DE l'ÉNERGIE NUCLÉAIRE
DIRECTION DU CENTRE DE CADARACHE
DÉPARTEMENT D'ÉTUDES DES RÉACTEURS
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Note Technique

TITRE : Trio_U Users Manual :
Methodology for incompressible single phase flow in industrial applications.

AUTEUR(S) : Ulrich Bieder, Valérie Barthel, Fréderic Ducros, Fabien Perdu, Patrick Quéméré.

RÉSUMÉ : Le code Trio_U est développé pour certains aspects de la thermohydraulique des écoulements mono- et multiphasique avec transfert de chaleur et de masse. Le présent document expose certaines modélisations numérique et physique référencées pour les applications industrielles en écoulement incompressible et monophasique en milieu libre. Il décrit assez précisément les équations résolues ainsi que les méthodes de résolution pour la discrétisation non-structurée en tétraèdre. Trois types d'application avec une modélisation de la turbulence adaptée sont ciblés dans le rapport et des exemples sont proposés pour chacun :

- Simulation des grandes échelles marginalement résolues par la méthode MILES
  - Simulation d'une grande partie d'un réacteur nucléaire
- Simulation des grandes échelles bien résolues par la méthode de viscosité turbulente
  - Simulation du refroidissement d'une cible de spallation
- Modélisation statistique de type « Reynolds Averaged Navier-Stokes equations » dit RANS
  - Expansion brusque d'un tube

Ce document concerne la version 1.5.3 de Trio_U et peut être considéré comme référence pour les versions à venir jusqu'à nouvel ordre.

MOTS CLÉS : Trio_U, methodology, LES, RANS, single phase flow

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List of Symbols

Capital letters

D	binary mass diffusivity	$m^2 \cdot s^{-1}$
F	external force	$kg \cdot m^{-1} \cdot s^{-1}$
G	term of buoyancy forces in k-ε model	$m^2 \cdot s^{-3}$
P	pressure	Pa
P_k	term of energy production in k-ε model	$m^2 \cdot s^{-3}$
S_i	source term of equation I	depending on equation
S	surface	m^2 in 2D, m^3 in 3D
S_{ij}	strain rate tensor	$m \cdot s^{-2}$
T	temperature	K
X	generic main unknown (u, T, Y)	depending on equation
Y	mass fraction together with $\sum_k Y_k = 1$	$kg \cdot kg^{-1}$

Small letters

c_p	heat capacity at constant pressure	$J \cdot kg^{-1} \cdot K^{-1}$
f_{vd}	van Driest dumping function	-
g	vector of gravity	$m \cdot s^{-2}$
k	turbulent kinetic energy	$m^2 \cdot s^{-2}$
k’	sub grid turbulent kinetic energy	$m^2 \cdot s^{-2}$
n	unit normal vector	-
q_x	flux density of x	$[x] \cdot m^{-2} s^{-1}$
t	time	s
u	vector of velocity	$m \cdot s^{-1}$
u^+	non dimensional velocity in wall units	-
u_τ	skin friction velocity	$m \cdot s^{-1}$
y^+	non dimensional wall coordinates	-

Greek letters

ε	rate of turbulent energy dissipation	$m^2 \cdot s^{-3}$
β_T	thermal expansion factor	K^{-1}
β_Y	mass expansion factor	-
μ	dynamic viscosity	$kg \cdot m^{-1} \cdot s^{-1}$
λ	thermal conductivity	$W \cdot m^{-1} \cdot K^{-1}$
τ	tensor viscous stress	$kg \cdot s^{-2}$
τ^R	Reynolds stress tensor	$kg \cdot s^{-2}$
τ^{SG}	sub grid stress tensor	$kg \cdot s^{-2}$
φ	heat flux density	$W \cdot m^{-2}$

κ	von Karman constant	-
ν	kinematic viscosity (μ/ρ)	$m^2 \cdot s^{-1}$
ρ	density	$kg \cdot m^{-3}$
Ω	volume of a control volume	m^2 in 2D, m^3 in 3D
ω	surface of a control volume	m in 2D, m^2 in 3D

Operators

Δ	difference
∇	gradient
$\nabla.$	divergence of a vector

Subscripts

f	fluid
f01	surface between points 0 and 1
k	tracer specie component k
m	momentum
th	thermal
s	solid
t	turbulent
w	wall
Y	tracer specie
0	reference value

Superscripts

p	iteration number p
p+1	iteration number p+1
t	actual time level t
t+1	new time level t+1
T	transposed
$\overline{x}$	Reynolds averaged mean value (RANS) or filtered value (LES) [1]
x’	fluctuating part after Reynolds decomposition or sub grid value (LES) [1]
0	reduced value

Non-dimensional numbers

Pr	Prandtl number
Pr_t	turbulent Prandtl number
Pr’	sub grid Prandtl number
Re	Reynolds number
Sc	Schmidt number
Sc_t	turbulent Schmidt number

[1] depending on the framework

Sc’ sub grid Schmidt number

1 Introduction

This document describes the mathematical modelling practices which are employed to selected models available in the Version 1.5.3 of the Trio_U thermal hydraulic code. The code was developed for the calculation of single- and multiphase fluid flow with heat and mass transfer within both an academic as well as an industrial environment. The mathematical modelling for incompressible single phase flows of industrial interest and the numerical solution technique employed to solve the model equations on non structured tetrahedral meshes are described in this report. We have primarily concentrated to describe “what” is calculated and have added information on “how” it is done (algorithm) only when necessary. More information on the algorithms will be presented in more detail in later “updated” versions of the document. Instructions and examples on the use of the code are added for three types of applications:

- Under resolved Large Eddy Simulation (LES) by using the MILES method
  - Simulation of an extended region of a nuclear reactor
- Resolved LES by using the eddy viscosity concept
  - Simulation of the cool ability of a tube like test section
- Statistical modelling of turbulence by means of “Reynolds Averages Navier-Stokes Equations” (RANS)
  - Simulation of an expanding tube

2 The general equations of Trio_U

The general equations which are treated by Trio_U for single phase thermal hydraulic problems are written in conservative form:

- The mass conservation

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho u) = 0$$

- The momentum conservation equations (Navier-Stokes equations)

$$\frac{\partial \rho u}{\partial t} + \nabla.(\rho uu) = -\nabla P + \nabla.(\tau) + F_m + S_m \quad \text{with:}$$

  - o $\tau = \mu(\nabla u + \nabla^T u - \frac{2}{3}\nabla.uI)$ for Newtonian fluids and
  - o $F_m = \rho g$ for gravitational forces
  - o S_m a momentum source term

- The conservation of the internal energy

$$c_p\left(\frac{\partial \rho T}{\partial t} + \nabla.(\rho uT)\right) = -\nabla.(q_{th}) + S_{th} + \frac{dP_{th}}{dt} \quad \text{with:}$$

  - o $q_{th} = -\lambda \nabla T$ Fourier's law of heat conduction
  - o S_{th} an energy source term
  - o P_{th} Thermodynamic pressure

- Equation for the conservation of k trace species

$$\frac{\partial \rho Y_k}{\partial t} + \nabla.(\rho u Y_k) = -\nabla.(q_{Yk}) + S_{Yk} \quad \text{with:}$$

  - o $q_{Yk} = -\rho \cdot D_{Yk} \nabla Y_k$ Fick's first law of binary diffusion
  - o S_{Yk} a tracer species source term

- Equation for heat conduction in solid structures

$$c_p\left(\frac{\partial \rho T}{\partial t}\right) = -\nabla.(q_{th}) + S_{th} \quad \text{with:}$$

  - o $q_{th} = -\lambda \nabla T$ Fourier's law of heat conduction
  - o S_{th} an energy source term

The reversible rate of internal energy change due to compression as well as viscous dissipation is not taken into account in the Energy equation. In the Diffusion equation, only ordinary diffusion is taken into account. Diffusion related to external forces and to the gradients of pressure and temperature is neglected It is self-evident that the fluid flow temperature can be coupled to heat conduction problems in solid structures

3 Simplifications for practical use

3.1 Quasi-compressible flow

The aim of the quasi-compressible model is to take into account the variation of the density due to the scalars (for example the temperature), and to avoid the difficulties met with description of a fully compressible flow; due to the compression effects acoustic waves propagate in the medium.

In the case of a low Mach number there is a large difference between the velocity of the flow and the velocity of acoustic waves. Then the time step of a numerical simulation of this kind of flow must be very small. In order to avoid this constraint an assumption may be applied to the pressure. The quasi-compressible model is based on a splitting of the pressure:

$$P(t,x) = P_{th}(t) + P_h(t,x)$$

With P_{th} denotes the thermodynamic pressure only time-dependent and P_h is the hydrodynamic pressure.

According to this splitting, the governing equations of the quasi-compressible flow implemented in Trio_U could be written :

- The mass conservation

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho u) = 0$$

- The momentum conservation equations (Navier-Stokes equations)

$$\frac{\partial \rho u}{\partial t} + \nabla.(\rho u u) = -\nabla P_h + \nabla.(\tau) + F_m + S_m$$ with:

  - o $\tau = \mu(\nabla u + \nabla^T u)$ for Newtonian fluids
  - o $F_m = \rho g$ for gravitational forces
  - o S_m a momentum source term

- The conservation of the internal energy

$$\rho c_p \left(\frac{\partial T}{\partial t} + u.\nabla T \right) = -\nabla.(q_{th}) + S_{th} + \frac{dP_{th}}{dt}$$ with:

  - o $q_{th} = -\lambda \nabla T$ Fourier's law of heat conduction
  - o S_{th} an energy source term
  - o P_{th} Thermodynamic pressure

The thermodynamic part P_{th} of the pressure is used in the equation of state in order to determine the density. For thermal-hydraulic flows, generally the law of state used in the Trio_U applicatiosn is the perfect gas law : $\rho(T) = \frac{P_{th}}{rT}$

Note: For more complex flows, for instance flows with transports of various scalar species, it is possible to use an well suited form of the equation of state. For the moment, these models are not presented in this report.

The thermodynamic pressure P_{th} can be computed by different ways in Trio_U :

- first, P_{th} can be chosen as an uniform field on the whole domain. This is the current option used in Trio_U

- P_{th} can be determined by a mass balance consideration. In this case, P_{th} is determined solving an ordinary differential equation. To obtain this equation, we differentiate the gas law using the continuity equation and balance equations :

$$\frac{1}{P_{th}}\frac{dP_{th}}{dt} = \frac{\int_V \frac{\rho}{T}\frac{\partial T}{\partial t} dV}{\int_V \rho dV}$$

3.2 Incompressible flow

It is assumed that the density of the fluid is constant ($\rho=\rho_0$). Thus the density is neither a function of the temperature nor of the composition of the fluid (fluid mixture). Buoyancy effects are taken into account only by gravitational forces. This simplification is known as Boussinesq approximation and is justified for $\Delta\rho/\rho_0 < 0.1$. The gravitational force is written for a non isothermal multi component mixture of trace species as

$$F_m = \rho_0 g + \left(\beta_T \cdot (T - T_0) + \sum_k \beta_{Y,k} \cdot (Y_k - Y_{k,0}) \right) \cdot \rho_0 g$$

- β_T is the thermal expansion coefficient of the fluid and
- $\beta_{Y,k}$ is the expansion coefficient due to the mixing of the tracer specie k.

The incompressibility assumption based on small temperature variations includes implicitly that the static pressure has no influence on the flow field:

$$\rho = \rho(T) \quad but$$
$$\rho \neq \rho(P)$$

Thus a reduced pressure is defined which includes the static pressure:

$$P^0 = \frac{P}{\rho_0} - g \cdot z$$

3.3 Temperature dependent physical properties

For the two presented options, it is assumed that the physical properties are independent of the local pressure. However, they can be a function of the local fluid temperature

- μ = $\mu(T)$
- λ = $\lambda(T)$
- D_{Yk} = $D_{Yk}(T)$
- c_p = const

In addition, in the quasi-compressible approach, the density can be dependent of the thermodynamic pressure, respect with for instance the perfect gas law.

3.4 Treatment of turbulent flow

Three different possibilities exist in Trio_U to simulate turbulent flow:

- Direct numerical simulation (DNS)
- Reynolds averaged Navier-Stokes equations (RANS)
- Large eddy simulations (LES)

3.4.1 Direct numerical simulation

The most exact approach to turbulence simulation is to solve the Navier-Stokes equations without any further approximations other than the numerical discretization. In such a simulation all motions contained in the flow are resolved. The simulation domain must be

- at least as large as the largest eddy in the system (integral scale)

and the meshing must be

- as fine as the dimension of the dissipating eddies (Kolomogorov scale)

3.4.2 Reynolds averaged equations

In this approach, the instationary velocity (u) can be written as the sum of a stationary (or very slowly varying) mean value $(\overline{u})$ and a time depending fluctuating quantity (u').

$$u = \overline{u} + u'$$

The conservation equations are written for the time averaged quantities (ensemble averaging for unsteady flow). Only the non-linear terms lead to contributions of the averaged quantities

on the fluctuating ones. These contributions must be modelled and are summarised and defined in the Reynolds stress tensors:

$$\tau^R = -\rho \cdot \overline{u'u'} = -\rho \cdot \left(\overline{u \cdot u} - \bar{u} \cdot \bar{u}\right)$$

Boussinesq's eddy viscosity concept relates the turbulent stresses to the gradients of the mean velocity (Boussinesq hypothesis):

$$-\rho \cdot \overline{u'u'} = \mu_T \cdot (\nabla \bar{u} + \nabla^T \bar{u}) - \frac{2}{3}\rho k \delta_{ij} .$$

The turbulent kinetic energy k is defined as: $k = 0.5 \cdot \overline{u_i' u_i'}$. This leads to the following viscous term in the Reynolds averaged Navier-Stokes equations (RANS) which includes both the molecular and turbulent contributions:

- Momentum equations

  $$\tau = (\mu + \mu_t) \cdot (\nabla \bar{u} + \nabla^T \bar{u} - \frac{2}{3} \nabla . \bar{u} I)$$

The same concept is used in analogy to the conservation of the energy and the tracer species:

- Energy conservation

  $q_{th} = -(\lambda + \lambda_t) \nabla \bar{T}$ with $\lambda_t = \frac{\mu_t}{\mathrm{Pr}_t}$

- Conservation of tracer species

  $q_{Yk} = -\rho \cdot (D_{Yk} + D_t) \nabla \bar{Y}_k$ with $D_t = \frac{\nu_t}{Sc_t}$

For most fluids $Pr_t = Sc_t = 0.9$. However, for fluids with low Pr numbers (liquid metals) Pr_t can be an analytical function of ν_t/Kays/:

$$\frac{\lambda_t}{\rho \cdot c_p} = \frac{\nu_t^2}{\left(0.7 \cdot \frac{\lambda}{\rho \cdot c_p} + 0.85 \cdot \nu_t\right)}.$$

Two approaches for industrial applications are used in the version 1.5.3 of Trio_U in order to determine the turbulent viscosity, conductivity and diffusivity; the mixing length model and the k-ε model.

3.4.2.1 The mixing length model

The mixing length approach is especially dedicated to simple wall bounded turbulence (as e.g. tube flow). The turbulent stresses are directly related to the mean velocity gradient normal to the wall.

$$-\rho \cdot \overline{u'u'} = \mu_T \cdot \nabla \bar{u}$$
$$\mu_T = \rho \cdot \kappa^2 \cdot l^2 \cdot \left| \frac{d\bar{u}}{dy} \right|$$

Here y is the wall normal direction and l is a prescribed function of the coordinates which stands for the distance to the wall.
For practical use, l is weighted with a van Driest type dumping function f_{vd}. In order to reduce the influence of l far from walls, another exponential function is added as described below. The model can then be written in a general form as a function of l_{max}, a user defined maximum distance from the wall:

$$\mu_T = \rho \cdot \left(f_{vd}^{\,2} \cdot \kappa \cdot l_m \right)^2 \cdot \sqrt{2 \cdot S_{ij}^{\,2}} \quad \text{with} \quad S_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad \text{and}$$

$$f_{vd} = 1 - \exp\left(\frac{-y^+}{A^+} \right) \qquad \text{with } A^+ = 26 \quad .$$

$$l_m = l \quad for \quad l \le l_{max}$$

$$l_m = l_{max} \cdot \exp\left(-2 \cdot \frac{l - l_{max}}{l_{max}} \right) \quad for \quad l > l_{max}$$

This model can be used in combination with both, wall functions (high Reynolds modelling) and no-slip boundary conditions (low Reynolds modelling). Particular formulations exist for tube and channel flows which are not described here.

3.4.2.2 The k-ε model

The high Reynolds form of the model is “appropriate” to fully developed turbulent flows /Launder/ and allows to some extent the presence of buoyancy effects /Viollet/. In the Boussinesq hypothesis framework, the turbulent viscosity is linked to the turbulent kinetic energy k and the dissipation rate of the turbulent kinetic energy ε via:

$$\mu_t = \rho \nu_t = C_\mu \frac{(\rho k)^2}{\rho \varepsilon}$$

Conservation equations are written for both the turbulent kinetic energy k and the turbulent dissipation rate ε.

- The conservation of the turbulence kinetic energy

$$\frac{\partial \rho k}{\partial t} + \bar{u}\nabla \rho k = \nabla.(\mu + \frac{\mu_t}{\sigma_k}\nabla k) - \rho\varepsilon + P + G$$

- The conservation of the turbulence dissipation rate

$$\frac{\partial \rho \varepsilon}{\partial t} + \bar{u}\nabla \rho \varepsilon = \nabla.(\mu + \frac{\mu_t}{\sigma_\varepsilon}\nabla \varepsilon) - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} + C_{\varepsilon 1}P\frac{\varepsilon}{k} + C_{\varepsilon 1}C_{\varepsilon 3}G\frac{\varepsilon}{k}$$

The production of turbulence kinetic energy is calculated by

$$P = -\overline{u_i' u_j'}\frac{\partial \bar{u}_i}{\partial x_j} \qquad \text{with} \qquad -\overline{u_i' u_j'} = \mu_t\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) - \frac{2}{3}\rho k \delta_{ij}$$

For quasi-compressible flows, G=0, buoyancy effects are directly treated by the intrinsic variation of the density.

For incompressible flows, buoyancy effects are treated by

$$G = -\frac{\nu_t}{\mathrm{Pr}_t}\beta_T g\nabla \bar{T} - \frac{\nu_t}{Sc_t}\beta_Y g\nabla \bar{Y},$$

The following empirical coefficients (Table 3.1) are used by default.

Table 3.1: Default coefficients of the standard high Reynolds number k-ε model

C_μ	σ_k	σ_ε	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	$C_{\varepsilon 3}$	Pr_t	Sc_t
0.09	1.0	1.3	1.44	1.92	1.0	0.9	0.9

To take into account the effect of thermal and concentration stratification, the following assumption is made /Viollet/:

$C_{\varepsilon 3}$ = 1 if G > 0 (stable stratification)
$C_{\varepsilon 3}$ = 0 if G < 0 (unstable stratification)

The coefficients have been defined experimentally and are thus dependant on the geometry. Especially the coefficient $C_{\varepsilon 3}$ depends on the ratio of the lift to convection. The product $C_{\varepsilon 1}C_{\varepsilon 3}$ increases with the Richardson number, this means with increasing influence of natural convection effects:

Table 3.2: Modification of the standard coefficients due to thermal effects

$C_{\varepsilon 3}$	**$C_{\varepsilon 1}$*$C_{\varepsilon 3}$**	**Configuration and reference**
1	$C_{\varepsilon 3}$	Flow near vertical heated wall /Launder/
0,56	0,8	Natural convection /Hanjalic/

0,63	0,91	Thermal instable mixing layer /Snider/

3.4.3 Large eddy simulation

The basic idea of LES is that the large turbulent structures efficiently transport the conserved properties whereas the smaller ones have a more general character and primarily dissipate the kinetic energy /Sagaut/. In order to separate the large-scale motions from the small-scale fluctuations, a filter operation is applied on the conservation equations. The instationary velocity (u) is written as the sum of a filtered value[2] $(\bar{u})$ and a fluctuating quantity (u').

$$u = \bar{u} + u'$$

In this filtering operation, only the non-linear terms lead to contributions of the unresolved scales to the resolved ones. These contributions must be modelled and are summarised and defined in the sub grid scale tensors:

$$\tau^S = -\rho \cdot \left(\overline{u \cdot u} - \bar{u} \cdot \bar{u} \right)$$

In analogy to the Boussinesq's eddy viscosity concept, the sub grid scale tensor is related to the large-scale strain tensor (written in filtered quantities).

$$-\rho \cdot \left(\overline{u \cdot u} - \bar{u} \cdot \bar{u} \right) = \mu_T \cdot (\nabla \bar{u} + \nabla^T \bar{u}) - \frac{2}{3} \rho k' \delta_{ij}$$

The sub grid turbulent kinetic energy k' is defined as: $k' = 0.5 \cdot (\overline{u_i \cdot u_i} - \bar{u}_i \cdot \bar{u}_i)$. This leads to the following viscous term in the filtered Navier-Stokes equation which includes both the molecular and turbulent contributions:

- Momentum equations

  $$\tau = (\mu + \mu_t) \cdot \left(\nabla \bar{u} + \nabla^T \bar{u} - \frac{2}{3} \nabla . \bar{u} I \right)$$

The same concept is used in analogy to the conservation of the energy and the tracer species:

- Energy conservation

  $q_{th} = -(\lambda + \lambda_t) \nabla \bar{T}$ with $\lambda_t = \frac{\nu_t}{\mathrm{Pr}'}$

- Conservation of tracer species

  $q_{Yk} = -\rho \cdot (D_{Yk} + D_t) \nabla \bar{Y}_k$ with $D_t = \frac{\nu_t}{Sc'}$

The sub grid Prandtl and Schmidt numbers Pr' and Sc' are usually taken identical to the turbulent Prandtl and Schmidt numbers Pr_t and Sc_t, respectively (see Table 3.1).

[2] In the LES framework, the over bar denotes filtered values not averaged values as in the RANS framework

3.4.3.1 Smagorinsky's model

This simple model is based on the Reynolds stress tensor of the resolved scales. The turbulent viscosity is calculated according to:

$$\mu_t = \rho\left(C_S \overline{\Delta}\right)^2 \cdot \sqrt{2 \cdot S_{ij} \cdot S_{ij}} \quad \text{where} \quad S_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right)$$

$\overline{\Delta}$ stands for the filter lengths which is calculated for each element (see §4.3) and Cs is the Smagorinsky constant (Cs=0.18).

3.4.3.2 The WALE model

This sub-grid model is based on two operators which are used to model the turbulent viscosity:

$$\mu_t = \rho\left(C_w \overline{\Delta}\right)^2 \cdot \frac{OP_1}{OP_2 + e} \quad \text{with} \quad Cw = 0.5 \quad \text{and} \quad e = 10^{-6}$$

$$OP_1 = \left(s_{ij}^d \cdot s_{ij}^d\right)^{3/2}$$

$$OP_2 = \left(S_{ij} \cdot S_{ij}\right)^{5/2} + \left(s_{ij}^d \cdot s_{ij}^d\right)^{5/4}$$

$$s_{ij}^d = \frac{1}{2} \cdot \left(g_{ij}^2 + g_{ij}^2\right) - \frac{1}{3} \cdot \delta_{ij} \cdot g_{kk}^2$$

$$S_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) \quad \text{and} \quad g_{ij} = \frac{\partial \overline{u}_i}{\partial x_j}$$

The model shows two properties which are very interesting for boundary layer flows: The turbulent viscosity tends to zero at the wall with the correct diminishing rate (~ y^3) and the model can predict the laminar turbulent transition.

3.5 Boundary conditions

The boundary conditions must cover the majority of physical situations. Any physically consistent mix of boundary conditions is admissible. The following conditions are usually used to describe industrial flows.

- Inflow (Dirichlet type)
  For inflow boundaries, it is assumed that the spatial and temporal distributions of the main unknowns are known.

- Outflow (von Neumann type)
  For outflow boundaries it is assumed that for all quantities, the gradients normal to the outflow plane are zero. The pressure distribution at this boundary is known.

- Impermeable Wall
  No-slip boundary conditions (adherence) are applied for the momentum equations at solid walls. Specific formulations are available especially in the case of turbulent flows. Either imposed values of the temperature or a concentration, respectively, or imposed heat- and mass fluxes are usually used for the energy and tracer specie transport equations.

- Slip surface
  This condition describes a moving non permeable wall or a moving free surface

- Symmetry
  This condition denotes a surface at which the normal velocity and the normal gradients of all other variables are zero.

- Cyclique Boundaries
  This boundary condition refers to a pair of surfaces at which the flow repeats itself either in terms of some variables or all variables.

4 The equations solved by Trio_U

4.1 The basic equations for quasi-compressible flows

Using the simplifications discussed above, the following conservation equations are solved by Trio_U for quasi-compressible fluids. In this section, we consider the case of a perfect gas and the only scalar specie is the temperature.

4.1.1 Laminar flow

- Equation of state

$$\rho = \frac{P_{th}}{rT}$$

- The mass conservation

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho u) = 0$$

- The Momentum conservation equations (Navier-Stokes equations)

$$\frac{\partial \rho u}{\partial t} + \nabla.(\rho uu) = -\nabla P_h + \nabla.(\tau) + g + S_m \quad \text{with}$$

  - $\tau = \mu\left(\nabla u + \nabla^T u\right)$ the tensor of viscous stresses
  - S_m for a momentum source term

- The conservation of the inner energy

$$\rho c_p\left(\frac{\partial T}{\partial t} + u.\nabla T\right) = -\nabla.(q_{th}) + S_{th} + \frac{dP_{th}}{dt}$$ with:

  - $q_{th} = -\lambda \nabla T$ Fourier's law of heat conduction
  - S_{th} an energy source term
  - P_{th} Thermodynamic pressure

4.1.2 Turbulent flow

Depending of the framework $\overline{u}$ stands for a mean value (RANS framework) or a filtered value (LES framework).

- Equation of state

$$\rho = \frac{P_{th}}{rT}$$

- The mass conservation

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho u) = 0$$

- The Momentum conservation equations (Navier-Stokes equations)

  $\frac{\partial \rho u}{\partial t} + \nabla.(\rho u u) = -\nabla P_h + \nabla.(\tau) + g + S_m$ with

  - $\tau = \mu \cdot \nabla \bar{u} + \mu_t \left(\nabla \bar{u} + \nabla^T \bar{u}\right)$ the tensor of turbulent stresses
  - S_m for a momentum source term

- The conservation of the inner energy

  $\rho c_p \left(\frac{\partial T}{\partial t} + u.\nabla T \right) = -\nabla.(q_{th}) + S_{th} + \frac{dP_{th}}{dt}$ with

  - $q_{th} = -(\lambda + \lambda_t)\nabla \bar{T}$ Fourier's law for turbulent flow
  - S_{th} for an energy source term

- The k and ε transport equations (RANS framework)

$$\frac{\partial \rho k}{\partial t} + \bar{u}\nabla \rho k = \nabla.(\mu + \frac{\mu_t}{\sigma_k}\nabla k) - \rho\varepsilon + P + G$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \bar{u}\nabla \rho \varepsilon = \nabla.(\mu + \frac{\mu_t}{\sigma_\varepsilon}\nabla \varepsilon) - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} + C_{\varepsilon 1}P\frac{\varepsilon}{k} + C_{\varepsilon 1}C_{\varepsilon 3}G\frac{\varepsilon}{k}$$

with P, G, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$ and $C_{\varepsilon 3}$ which are given by the standard model (§2.4.2) with:

$C_{3local} = C_{\varepsilon 3}$	if	G<= 0	so	$C_{\varepsilon 3} = 0$	if	G<= 0 ;
$C_{3local} = 0$	if	G > 0	so	$C_{\varepsilon 3} = 1$	if	G>0.

In the VEF discretisation, the trace of the Reynolds stress tensor ($2/3 \cdot k \cdot \delta_{ij}$) is not taken into account in the production term *P*.

4.2 The basic equations for incompressible flows

Using the simplifications discussed above, the following conservation equations are solved by Trio_U for incompressible fluids. However, certain operators are based on additional hypotheses. These hypotheses as well as the resulting term in the conservation equation are discussed in the chapter "numerical scheme".

4.2.1 Laminar flow

- The mass conservation

$$\nabla.u = 0$$

- The Momentum conservation equations (Navier-Stokes equations)

$$\frac{\partial u}{\partial t} + \nabla.(uu) = -\nabla P^0 + \nabla.(\tau^0) + F^0{}_m + S^0{}_m \text{ with}$$

  - o $\tau^0 = \frac{\mu}{\rho_0}\nabla u$ the tensor of viscous stresses
  - o $P^0 = \frac{P}{\rho_0} - g \cdot z$ the reduced pressure term
  - o $F^0{}_m = \left(\beta_T \cdot (T - T_0) + \beta_Y \cdot (Y - Y_0)\right) \cdot g$ for gravitational forces (binary mixture)
  - o $S^0{}_m = S_m/\rho_0$ for a momentum source term

- The conservation of the inner energy

$$\frac{\partial T}{\partial t} + \nabla.(uT) = -\nabla.(q^0{}_{th}) + S^0{}_{th} \quad \text{with}$$

  - o $q^0{}_{th} = -\frac{\lambda}{\rho_0 \cdot c_p}\nabla T$ Fourier's law
  - o $S^0_{th} = S_{th}/(\rho\, c_p)$ for an energy source term
  - o $\nabla.(uT) = 0$ for heat conduction in solid structures

- Equation for the conservation of k trace species

$$\frac{\partial Y_k}{\partial t} + \nabla.(uY_k) = -\nabla.(q^0{}_{Yk}) + S^0{}_{Yk} \quad \text{with}$$

  - o $q^0{}_{Yk} = -D \cdot \nabla Y_k$ Fick's law
  - o $S^0_{Yh} = S_{Yh}/\rho_0$ for a traces species source term

4.2.2 Turbulent flow

Depending of the framework $\bar{u}$ stands for a mean value (RANS framework) or a filtered value (LES framework).

- The mass conservation

$$\nabla.\bar{u} = 0$$

- The Momentum conservation equations (Navier-Stokes equations)

$$\frac{\partial \bar{u}}{\partial t} + \nabla.(\bar{u}\bar{u}) = -\nabla P^0 + \nabla.(\tau^0) + F^0{}_m + S^0{}_m \text{ with}$$

  - $\tau^0 = \frac{\mu}{\rho_0} \cdot \nabla \bar{u} + \nu_t (\nabla \bar{u} + \nabla^T \bar{u})$ the tensor of turbulent stresses
  - $P^0 = \frac{P}{\rho_0} - g \cdot z$ the reduced pressure term
  - $F^0{}_m = (\beta_T \cdot (\bar{T} - \bar{T}_0) + \beta_Y \cdot (\bar{Y} - \bar{Y}_0)) \cdot g$ for gravitational forces (binary mixture)
  - $S^0{}_m = S_m/\rho_0$ for a momentum source term

- The conservation of the inner energy

$$\frac{\partial \bar{T}}{\partial t} + \nabla.(\bar{u}\bar{T}) = -\nabla.(q^0{}_{th}) + S^0{}_{th} \quad \text{with}$$

  - $q^0{}_{th} = -\frac{\lambda + \lambda_t}{\rho_0 \cdot c_p} \nabla \bar{T}$ Fourier's law for turbulent flow
  - $S^0{}_{th} = S_{th}/(\rho\, c_p)$ for an energy source term

- Equation for the conservation of k trace species

$$\frac{\partial \bar{Y}_k}{\partial t} + \nabla.(\bar{u}\bar{Y}_k) = -\nabla.(q^0{}_{Yk}) + S^0{}_{Yk} \quad \text{with}$$

  - $q^0{}_{Yk} = -(D + D_t) \nabla \bar{Y}_k$ Fick's law for turbulent flow
  - $S^0{}_{Yh} = S_{Yh}/\rho_0$ for a traces species source term

- The k and ε transport equations (RANS framework)

$$\frac{\partial k}{\partial t} + \nabla.(\bar{u}k) = \nabla.(\frac{\nu_t}{\sigma_k} \nabla k) - \varepsilon + P + G$$

$$\frac{\partial \varepsilon}{\partial t} + \nabla.(\bar{u}\varepsilon) = \nabla.(\frac{\nu_t}{\sigma_\varepsilon} \nabla \varepsilon) - C_{\varepsilon 2} \frac{\varepsilon^2}{k} + C_{\varepsilon 1} P \frac{\varepsilon}{k} + C_{\varepsilon 1}(1 - C_{3local}) G \frac{\varepsilon}{k}$$

with P, G, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$ and $C_{\varepsilon 3}$ which are given by the standard model (§2.4.2) with:

$C_{3local} = C_{\varepsilon 3}$ if $G <= 0$ so $C_{\varepsilon 3} = 0$ if $G <= 0$;

$C_{3local} = 0$ if $G > 0$ so $C_{\varepsilon 3} = 1$ if $G>0$.

In the VEF discretisation, the trace of the Reynolds stress tensor ($2/3 \cdot k \cdot \delta_{ij}$) is not taken into account in the production term *P*.

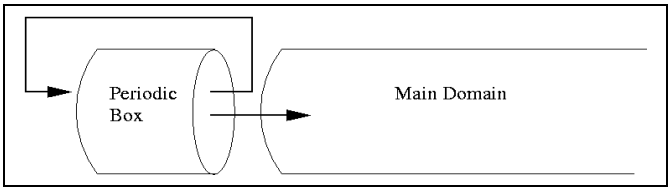
4.3 Boundary conditions

4.3.1 Inflow (Dirichlet type)

For inflow boundaries, it is assumed that the spatial and temporal distributions of the main unknowns are known. These unknowns can be either instantaneous averaged or filtered quantities. The following variables are thus imposed at the inflow faces:

- All vector components of the velocity[3]
- The temperature
- The tracer species concentration

- In order to impose turbulent velocity fluctuations in LES calculations, a "simple" procedure is recommended which is based on the use of periodic tubes, which in their turn are located at the domain inlets.



- Simple estimations are usually sufficient for the properties of k-ε turbulence modelling:

$$k = \frac{1}{2}(u')^2 \quad where \quad u' \approx 0.1 \cdot u$$

$$\varepsilon = \frac{C_\mu^{3/4} \cdot k^{3/2}}{l}$$

Plausible values of the characteristic integral mixing length l can be estimated form the global geometry (for example hydraulic diameter).

4.3.2 Outflow (von Neumann type)

For outflow boundaries it is assumed that for all quantities, the gradients normal to the outflow plane are taken to be zero. The exit mass flow is fixed from overall continuity

[3] Mass fluxes must be imposed as velocity

consideration. For the momentum equation, this “free out-stream” condition is assured by an imposed pressure.

4.3.3 Symmetry

This condition denotes a surface at which the normal velocity and the normal gradients of all other variables are zero. There is no flux across the surface.

4.3.4 Periodic Boundaries

This boundary condition refers to a pair of surfaces at which the flow repeats itself either in terms of some variables or all variables. The meshing of both surfaces must be identical.

4.3.5 Wall

Specific boundary conditions are applied for solid walls, especially in the case of turbulent flows.

4.3.5.1 Velocity

Adherence

The no slip boundary condition (u=0) is used in the case of laminar flow or in the case of wall resolved turbulent flow.

Wall functions

In this approach, algebraic relations based on the known distribution of the velocity[4] in a one-dimensional equilibrium flow are used to “bridge” the boundary layer. Based on the normalized wall quantities,

$$u_+ = u/u_\tau$$
$$y^+ = \rho \cdot y \cdot u_\tau / \mu$$

Reichardt has proposed the following general law,

$$u^+ = \frac{1}{\kappa} \cdot \ln\left(1+\kappa \cdot y^+\right) + 7.8 \cdot \left[1 - \exp\left(-\frac{y^+}{11}\right) - \frac{y^+}{11}\exp\left(-0.33 y^+\right)\right],$$

which describes the flow field in all boundary layer regions. The wall friction finally defines the momentum flux at the wall which used in the diffusion operators

$$\rho \cdot u_\tau^{\,2} = \mu \cdot \left.\frac{\partial u}{\partial n}\right|_w \quad .$$

4.3.5.2 Temperature

Imposed temperature

[4] In order to simplify the notation, the velocity u can be either a mean value (RANS framework) or a filtered value (LES framework)

- In wall resolved simulations, the temperature of the wall is directly imposed.
- When using wall functions, an algebraic relation based on the known distribution of the temperature in a one-dimensional flow is used to "bridge" the boundary layer. Kader has proposed such a general bridging formulation:

$$\varphi_w = \lambda_f \frac{T_f - T_w}{d_{eq}} \qquad \text{with} \quad d_{eq} = T^+ \frac{\lambda_f}{\rho \cdot c_p \cdot u_\tau}$$

$$T^+\left(y^+, \mathrm{Pr}\right) = \mathrm{Pr} \cdot y^+ \cdot e^{\Gamma} + \left(2.12 \cdot \ln\left(1 + y^+\right)\right) \cdot e^{-1/\Gamma} \qquad \text{with} \quad \Gamma = \frac{0.01 \cdot \left(\mathrm{Pr} \cdot y^+\right)^4}{1 + 5 \cdot \mathrm{Pr}^3 \cdot y^+}$$

Imposed flux

A temporal and special varying distribution of a heat flux density can be imposed on the walls. In this case, the wall temperature is not used in the calculation; however it can be post processed.

Adiabatic

This is the boundary condition for simulating perfectly isolated walls. It denotes a surface at which the normal gradient of the temperature is zero.

Heat exchange between solid wall and fluid flow (conjugated heat transfer)

At the interface which couples the heat exchange between a solid wall and the fluid flow, the thermal fluxes equality between a fluid (f) and a solid (s) is expressed as:

$$\varphi_f = \varphi_s \quad \Rightarrow \quad \lambda_f \left.\frac{\partial T_f}{\partial n}\right|_w = -\lambda_s \left.\frac{\partial T_s}{\partial n}\right|_w$$

λ refers to the thermal conductivity and n, is the normal vector at the wall/fluid interface (exterior to the considered domain).

4.3.5.3 Concentration

For tracer species, impermeable walls are used, for which the concentration gradient normal to the wall is zero.

4.3.5.4 Turbulent kinetic energy and dissipation

Under equilibrium conditions (the production of turbulent kinetic energy is equal to the dissipation of turbulent kinetic energy), the following boundary conditions are used for walls:

$$k^+ = C_\mu^{-0.5} \quad where \quad k^+ = \frac{k \cdot \rho}{\tau_w}$$

$$\varepsilon^+ = C_\mu^{3/4} \Big/ \kappa \quad where \quad \varepsilon^+ = \frac{\varepsilon \cdot y_p}{k^{3/2}}$$

Here, y_p is the distance from the wall to the first wall near point.

Note that for the quasi-compressible case, the boundary conditions concern the quantities ρk and $\rho\varepsilon$.

4.4 The characteristic filter length of the meshing

The characteristic filter length $\overline{\Delta}$ is calculated for each tetrahedron of the meshing from the volume of the tetrahedron:

$$\overline{\Delta} = \sqrt[3]{volume\ of\ \ tetra}$$

In order to avoid in a heterogeneous meshing very strong variations of the filter length from one tetra to the next, a two step smoothing procedure is applied to the filter length of each element:

- Firstly, to each vertex of the meshing is associated the maximum filter length of all connected tetrahedrons:

  $$\overline{\Delta}_{vertex} = \max(\overline{\Delta}_i), \quad \text{for i = 1, elem}$$

  "elem" describes all elements which are connected to a specific vertex.

- Secondly, to each tetrahedron of the meshing is re-associate the maximum filter length of all connected vertices:

  $$\overline{\Delta} = \max(\overline{\Delta}_j), \ \text{j=1, vertex}$$

  "vertex" describes the four corners of the tetra for which the filter length is calculated.

5 Differential equations in discrete space

The numerical model is based on a finite volume method. The conservation equations are used in conservative form and are integrated over a (control) volume Ω, which is bounded by the surface ω. Applying Gauss' theorem leads for the Navier-Stokes equations to the following system of equations for laminar flow:

- the mass conservation:

$$\int_{\omega} u_i n_i \, ds = 0$$

- the momentum conservation

$$\int_{\Omega} \frac{\partial u_i}{\partial t} dV + \int_{\omega} u_i u_j n_j \, ds = \int_{\omega} 2 \cdot \nu \cdot S_{ij} n_j \, ds + \int_{\omega} P^0 n_j \, ds + \int_{\Omega} F_{m,i} \, dV$$

Using Einstein's notation n_i is a component of the normal unity vector of ω which is oriented to the external side of Ω. The kinematic viscosity ν can be a function of the temperature. For turbulent flow, the Navier-Stokes equations are written:

- the mass conservation:

$$\int_{\omega} \overline{u}_i n_i \, ds = 0$$

- the momentum conservation

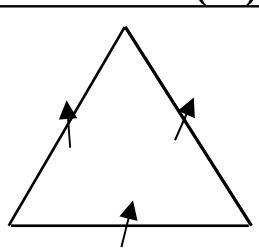
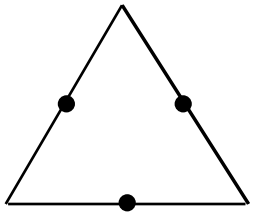
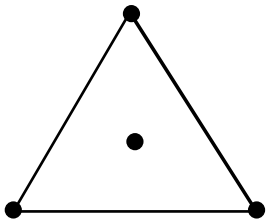
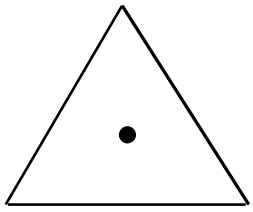
$$\int_{\Omega} \frac{\partial \overline{u}_i}{\partial t} dV + \int_{\omega} \overline{u}_i \overline{u}_j n_j \, ds = \int_{\omega} 2 \cdot (\nu + \nu_t) \cdot S_{ij} n_j \, ds + \int_{\omega} P^0 n_j \, ds + \int_{\Omega} F_{m,i} \, dV$$

The "over bar" stands for mean values in the RANS framework and for filtered values in the LES framework.

5.1 Discretisation

The discretisation is done on a tetrahedral mesh by using a hybrid finite element/finite volume discretisation method. In this method, the volume integrals as well as the fluxes crossing the surface of a control volume are evaluated by using the finite element technique that is by means of the form functions of the element. The used elements and the associated localisation of the unknowns are summarised on Table 5.1. The given form functions are used to determine the distribution of the unknowns on each location of an element /Heib/, /Fortin/.

Table 5.1: Summery of the discretisation method

Quantity	Form function	Localisation	Visualisation (2D)
Vectors: Velocity	P1 non conforming: Linear in element	Centre of faces (not centre of edges)	
Scalars I: Temperature Concentration k and ε	P1 non conforming: Linear in element	Centre of faces (not centre of edges)	
Scalar II: Pressure	P1/P0: Linear in the element and Constant per element	In the vertices and in the centre of the element	
Physical properties I: Viscosity Conductivity Diffusivity	P0: Constant per element[5]	In the centre of the element	
Physical properties II: Density Heat capacity Expansion coefficient	P0: Constant per element	In the centre of the element	

5.2 Temporal integration of the conservation equations

Three different classes of time integrating methods /Ferziger/ exist in Trio_U to calculate the main unknowns[6] for the time level t+dt, abbreviated by “t+1”, starting from known values at the time level “t”: the explicit scheme, the semi implicit scheme and the implicit scheme. It is important to note that only one time scheme is applied for the integration of the whole problem. This is also true for coupled problems (conjugated heat transfer). However, two different problems can be integrated by two different time schemes.

[5] Calculated from the mean temperature of the element
[6] The unknowns can be instantaneous values, mean values (RANS) or filtered values (LES)

The following two basic hypotheses are used in all time schemes to integrate the conservation equations from the time level t to t+1:

- The physical properties as well as all source terms are evaluated for the time level t and are kept constant for the integration.
- The boundary conditions are taken at the time level t and are kept constant during the integration.

5.2.1 The SOLA solution algorithm for the momentum equation

The SOLA algorithm /Hirt/ is used to integrate the Navier-Stokes equations. Knowing a velocity field u with $\nabla.u = 0$, this algorithm computes the pressure field P and the associated time derivative $\partial u / \partial t$ in such a way that $\nabla.(\partial u / \partial t) = 0$. The pressure is taken implicitly in the momentum equations and the velocities are taken implicitly in the continuity equation. All other terms are taken explicitly. The resulting conservation equations are then written in matrix form:

$$M \frac{\partial u}{\partial t} = A \cdot u + L(u) \cdot u + B^T P + S$$
$$B \cdot \frac{\partial u}{\partial t} = 0$$

where the following matrix operators are defined ;

- A = Matrix operator of the diffusion
- L(u) = Matrix operator of the convection
- B = Matrix operator of the divergence
- B^T = Matrix operator of the gradient
- M = Matrix operator of the « diagonal mass »
- S = Source term (sum of further volume forces)

Multiplying the momentum equation by BM^{-1} cancels its left hand side due to the mass conservation condition:

$$BM^{-1} \cdot \left(A \cdot u + L(u) \cdot u + B^T P + S \right) = 0$$

Then the following Poisson equation for the pressure

$$BM^{-1} B^T P = -BM^{-1} \cdot \left(A \cdot u + L(u) \cdot u + S \right) ,$$

which has the form of a Laplace operator, is used to calculate a pressure field, which allows to get a divergence-free time derivative $\partial u / \partial t$. The explicit and semi implicit time schemes presented below call the SOLA algorithm with the unknowns at different time levels.

5.2.2 Explicit time schemes

In the explicit time schemes only the mass conservation and the pressure gradient (more precisely the gradient of the reduced pressure P^0) are calculated with their unknowns at the time level "t+1" (t+Δt).

5.2.2.1 First order Euler forward scheme

The first order scheme is based on a first order forward time difference, which, in the case of the momentum equation, results from the SOLA algorithm

$$u^{t+1} = u^t + \Delta t \cdot \left.\frac{\partial u}{\partial t}\right|_{SOLA}^{t}$$

Two further hypotheses are used to integrate the conservation equations from the time level t to t+1:

- None of the main unknowns are updated when available for other equations.
- The turbulence models and their associated equations as well as all supplementary functions (as e.g. the wall functions) are solved by using all the variables at initial time level t.

The following equations are treated with quantities at the noted time levels:

- The mass conservation
$$\nabla . u^{t+1} = 0$$

- The Momentum conservation equations
$$\frac{u^{t+1} - u^t}{\Delta t} + \nabla . \left(u^t u^t\right) = -\nabla P^{0,t+1} + \nabla . \left(\tau^{0,t}\right) + F^{0,t}{}_m + S^{0,t}{}_m$$

- The conservation of the inner energy
$$\frac{T^{t+1} - T^t}{\Delta t} + \nabla . \left(u^t T^t\right) = -\nabla . \left(q^{0,t}{}_{th}\right) + S^{0,t}{}_{th}$$

- Equation for the conservation of k trace species
$$\frac{Y_k{}^{t+1} - Y_k{}^t}{\Delta t} + \nabla . \left(u^t Y_k{}^t\right) = -\nabla . \left(q^{0,t}{}_{Yk}\right) + S^{0,t}{}_{Yk}$$

- Conduction in solid structures
$$\frac{T^{t+1} - T^t}{\Delta t} = -\nabla . \left(q^{0,t}{}_{th}\right) + S^{0,t}{}_{th}$$

5.2.2.2 Third order Runge-Kutta scheme

For the Runge-Kutta scheme of 3rd order accuracy, three successive predictor-corrector steps must be achieved. The SOLA algorithm is called in any predictor-corrector step of the momentum equations in order to assure a divergence free velocity field in all sub-steps. Two further hypotheses are used to integrate the conservation equations from the time level t to t+1:

- None of the main unknowns are updated when available for other equations.
- The turbulence models and their associated equations as well as all supplementary functions (as e.g. the wall functions) are solved by using the variables at corrector time levels t+1/3 and t+3/4.

The following equations are treated with quantities at the noted time levels:

- The Momentum conservation equation

$$u^{t+1/3} = u^t + \frac{1}{3}\Delta t \cdot \left(-\nabla.u^t u^t - \nabla P^{0,t+1/3} + \nabla.\left(\tau^{0,t}\right) + F_m^{0,t} + S^{0,t}\right)$$

$$u^{t+3/4} = u^t + \frac{3}{4}\Delta t \cdot \left(-\frac{1}{4}\cdot\left(-\nabla.u^t u^t - \nabla P^{0,t+1/3} + \nabla.\left(\tau^{0,t}\right) + F_m^{0,t} + S^{0,t}\right) + \frac{4}{5}\cdot\left(-\nabla.u^{t+1/3}u^{t+1/3} - \nabla P^{0,t+3/4} + \nabla.\left(\tau^{0,t+1/3}\right) + F_m^{0,t} + S^{0,t}\right)\right)$$

$$u^{t+1} = u^t + \Delta t \cdot \left(-\frac{1}{6}\cdot\left(-\nabla.u^t u^t - \nabla P^{0,t+1/3} + \nabla.\left(\tau^{0,t}\right) + F_m^{0,t} + S^{0,t}\right) + \frac{3}{10}\cdot\left(-\nabla.u^{t+1/3}u^{t+1/3} - \nabla P^{0,t+3/4} + \nabla.\left(\tau^{0,t+1/3}\right) + F_m^{0,t} + S^{0,t}\right) + \frac{8}{15}\cdot\left(-\nabla.u^{t+3/4}u^{t+3/4} - \nabla P^{0,t+1} + \nabla.\left(\tau^{0,t+3/4}\right) + F_m^{0,t} + S^{0,t}\right)\right)$$

- The conservation of the inner energy

$$T^{t+1/3} = T^t + \frac{1}{3}\Delta t \cdot \left(-\nabla.u^t T^t - \nabla.\left(q_{th}^{0,t}\right) + S_{th}^{0,t}\right)$$

$$T^{t+3/4} = T^t + \frac{3}{4}\Delta t \cdot \left(-\frac{1}{4}\cdot\left(-\nabla.u^t T^t - \nabla.\left(q_{th}^{0,t}\right) + S_{th}^{0,t}\right) + \frac{4}{5}\cdot\left(-\nabla.u^t T^{t+1/3} - \nabla.\left(q_{th}^{0,t+1/3}\right) + S_{th}^{0,t}\right)\right)$$

$$T^{t+1} = T^t + \Delta t \cdot \left(-\frac{1}{6}\cdot\left(-\nabla.u^t T^t - \nabla.\left(q_{th}^{0,t}\right) + S_{th}^{0,t}\right) + \frac{3}{10}\cdot\left(-\nabla.u^t T^{t+1/3} - \nabla.\left(q_{th}^{0,t+1/3}\right) + S_{th}^{0,t}\right) + \frac{8}{15}\cdot\left(-\nabla.u^t T^{t+3/4} - \nabla.\left(q_{th}^{0,t+3/4}\right) + S_{th}^{0,t}\right)\right)$$

- The conservation of the tracer specie k

$$Y_k^{t+1/3} = Y_k^t + \frac{1}{3}\Delta t \cdot \left(-\nabla.u^t Y_k^t - \nabla.\left(q_{Yk}^{0,t}\right) + S_{Yk}^{0,t}\right)$$

$$Y_k^{\,t+3/4} = Y_k^{\,t} + \frac{3}{4}\Delta t \cdot \left(-\frac{1}{4} \cdot \left(-\nabla.u^t Y_k^{\,t} - \nabla.\left(q_{Yk}^{0,t}\right) + S_{Yk}^{0,t} \right) + \frac{4}{5} \cdot \left(-\nabla.u^t Y_k^{\,t+1/3} - \nabla.\left(q_{Yk}^{0,t+1/3}\right) + S_{Yk}^{0,t} \right) \right)$$

$$Y_k^{\,t+1} = Y_k^{\,t} + \Delta t \cdot \left(-\frac{1}{6} \cdot \left(-\nabla.u^t Y_k^{\,t} - \nabla.\left(q_{Yk}^{0,t}\right) + S_{Yk}^{0,t} \right) + \frac{3}{10} \cdot \left(-\nabla.u^t Y_k^{\,t+1/3} - \nabla.\left(q_{Yk}^{0,t+1/3}\right) + S_{Yk}^{0,t} \right) + \frac{8}{15} \cdot \left(-\nabla.u^t Y_k^{\,t+3/4} - \nabla.\left(q_{Yk}^{0,t+3/4}\right) + S_{Yk}^{0,t} \right) \right)$$

5.2.3 Semi implicit time scheme

The semi implicit time scheme is based on a fractional steps method which is associated to the 1st order Euler explicit time scheme and is only applicable with this scheme. Besides the mass conservation and the pressure gradient, the diffusion terms are calculated with their values at t+dt, abbreviated by "t+1". Two further hypotheses are used to integrate the conservation equations from the time level t to t+1:

- None of the main unknowns are updated when available for other equations.
- The turbulence models and their associated equations as well as all supplementary functions (as e.g. the wall functions) are solved by using all the variables at initial time level t.

The following equations are treated with quantities at the noted time levels:

- The mass conservation
$$\nabla.u^{t+1} = 0$$

- The Momentum conservation equations
$$\frac{u^{t+1} - u^t}{\Delta t} + \nabla.\left(u^t u^t\right) = -\nabla P^{0,t+1} + \nabla.\left(\tau^{0,t+1}\right) + F^{0,t}{}_m + S^{0,t}{}_m$$

- The conservation of the inner energy
$$\frac{T^{t+1} - T^t}{\Delta t} + \nabla.\left(u^t T^t\right) = -\nabla.\left(q^{0,t+1}{}_{th}\right) + S^{0,t}{}_{th}$$

- Equation for the conservation of k trace species
$$\frac{Y_k^{\,t+1} - Y_k^{\,t}}{\Delta t} + \nabla.\left(u^t Y_k^{\,t}\right) = -\nabla.\left(q^{0,t+1}{}_{Yk}\right) + S^{0,t}{}_{Yk}$$

- Conduction in solid structures
$$\frac{T^{t+1} - T^t}{\Delta t} = -\nabla.\left(q^{0,t+1}{}_{th}\right) + S^{0,t}{}_{th}$$

The semi implicit scheme is activated in the Euler explicit time scheme by using the keyword "diffusion_semi_implicite"

5.2.4 Implicit time scheme

In the implicit time scheme, all terms of the conservation equations are calculated with quantities which represent more actual time levels.

5.2.4.1 First order Euler backward scheme

The 1st order Euler backward implicit time scheme is solved either with the PISO algorithm or with SIMPLER algorithm.

$$u^{t+1} = u^{t} + \Delta t \cdot \left.\frac{\partial u}{\partial t}\right|_{PISO\,/\,SIMPLER}^{t+1}$$

Based on two further hypotheses, the conservation equations are integrated from the time level t to t+1:

- The main unknowns are updated for other equations as soon as available.
- The turbulence models and their associated equations as well as all supplementary functions (as e.g. the wall functions) are solved by using all the variables at initial time level t. As a consequence, the (turbulent) diffusivity is taken from the time level t even though the velocities are taken from the time level t+1!

The following equations are treated with quantities at the noted time levels:

- The mass conservation
$$\nabla . u^{t+1} = 0$$

- The Momentum conservation equations
$$\frac{u^{t+1} - u^{t}}{\Delta t} + \nabla . \left(u^{t+1} u^{t+1}\right) = -\nabla P^{0,t+1} + \nabla . \left(\tau^{0,t+1}\right) + F^{0,t}{}_{m} + S^{0,t}{}_{m}$$

- The conservation of the inner energy
$$\frac{T^{t+1} - T^{t}}{\Delta t} + \nabla . \left(u^{t+1} T^{t+1}\right) = -\nabla . \left(q^{0,t+1}{}_{th}\right) + S^{0,t}{}_{th}$$

- Equation for the conservation of k trace species
$$\frac{Y_k{}^{t+1} - Y_k{}^{t}}{\Delta t} + \nabla . \left(u^{t+1} Y_k{}^{t+1}\right) = -\nabla . \left(q^{0,t+1}{}_{Yk}\right) + S^{0,t}{}_{Yk}$$

- Conduction in solid structures
$$\frac{T^{t+1} - T^{t}}{\Delta t} = -\nabla . \left(q^{0,t+1}{}_{th}\right) + S^{0,t+1}{}_{th}$$

5.2.4.2 Second order Crank Nicholson scheme

In the algorithm recommended for LES calculations (keyword Sch_CN_EX_iteratif) the Crank-Nicholson method is used only to integrate the momentum equations. It is of second order accuracy for the Navier-Stokes equations and is based on the mid-point rule formulation (so called Euler-centred scheme /Ferziger/)

$$u^{t+1/2} = u^t + \frac{\Delta t}{2} \cdot \left.\frac{du}{dt}\right|_{t+1/2}$$
$$u^{t+1} = u^t + \Delta t \cdot \left.\frac{du}{dt}\right|_{t+1/2}$$

One further hypothesis is needed to integrate the conservation equations from the time level t to t+1:

- The turbulence models and their associated equations as well as all supplementary functions (as e.g. the wall functions) are solved by using all the variables at initial time level t. As a consequence, the (turbulent) diffusivity is taken from the time level t even though the velocities are taken from the time level t+1/2!

The solved mass and momentum conservation equations as well as the associated time levels are written below:

- The mass conservation

$$\nabla . u^{t+1/2} = 0$$
$$\nabla . u^{t+1} = 0$$

- The momentum conservation equations

$$\frac{u^{t+1/2} - u^t}{\Delta t / 2} + \nabla . \left(u^{t+1/2} u^{t+1/2}\right) = -\nabla P^{0,t+1/2} + \nabla . \left(\tau^{0,t+1/2}\right) + F^{0,t}{}_m + S^{0,t}{}_m$$
$$\frac{u^{t+1} - u^t}{\Delta t} + \nabla . \left(u^{t+1/2} u^{t+1/2}\right) = -\nabla P^{0,t+1} + \nabla . \left(\tau^{0,t+1/2}\right) + F^{0,t}{}_m + S^{0,t}{}_m$$

An estimation of the time derivative du/dt at the time level t+1/2 is obtained by an iterative method which is based on a Jacobi algorithm with under-relaxation. In order to assure the mass conservation, the SOLA algorithm is called within these iteration loop. This algorithm is stable only if Δt/2 is less than the Fourier limit. Bigger time steps can be achieved by using a relaxation factor. The iterations are repeated until the following convergence criterion is achieved:

$$\frac{\max \left\| u^{p+1} - u^p \right\|_\Omega}{\max \left\| u^p \right\|_\Omega} \leq threshold$$

In order to reduce the number of iterations per time step, the time step is dynamically adapted as a function of the number of p-iterations necessary to reach convergence.

The scalar quantities temperature and trace specie are treated outside the Crank-Nicholson scheme by n Euler explicit sub-steps (n is a pair number) which again respect the CFL and Fourier stability criteria. Neither the velocity nor the physical properties are updated for these equations.

- The conservation of the inner energy

$$T^{t+1} - T^{t} = \sum_{i=0}^{n} \left(- \nabla .\left(u^{t} T^{t+i} \right) - \nabla .\left(q^{0,t}{}_{th} \right) + S^{0,t}{}_{th} \right) \cdot \Delta t_i$$

- Equation for the conservation of k trace species

$$Y_k{}^{t+1} - Y_k{}^{t} = \sum_{i=0}^{n} \left(- \nabla .\left(u^{t} Y_k{}^{t+i} \right) - \nabla .\left(q^{0,t}{}_{Yk} \right) + S^{0,t}{}_{Yk} \right) \cdot \Delta t_i$$

For conjugated heat transfer problems, both domains (fluid and solid) are treated alternating until the overall convergence is obtained.

A more general formulation of overall 2nd order accuracy is available where both the momentum equations and the scalar transport equations are treated within the Crank Nicholson algorithm described above (keyword Sch_CN_iterative). In this case, the main unknowns are updated when available for other equations. However, the solution algorithm might lead to numerical instabilities.

5.3 Integration of the conservation equation in space

5.3.1 Convection term

5.3.1.1 Conservative finite volume formulation

In these types of schemes, the convective fluxes are calculated according to the conservative divergence formulation $\nabla .(uu)$ for the momentum equations or according to $\nabla .(uX)$ for the scalar quantity X. In the finite volume framework this leads to:

$$\int_{\Omega} \nabla .(uX) \cdot dV = \int_{\omega} uX \cdot dS = \sum_{fij} \mu X \cdot S_{fij}$$

The prediction of the fluxes is based on the discrete P1 non conforming representation of the velocity and scalar flow fields on the meshing. Here fij expresses the faces of the control volume around Fi, the location of a main unknown of the conservation equations. In Figure 5.1, the control volume for the unknown at F_0, located in the centre of the face, is represented by the points S_1, C_1, S_2 and C_2. In this context, S_i represent the vertices and C_i the centres of gravity of the elements E_i

Ex = Element number x
Sx = Vertex number x
Cx = Center of gravity of Ex
Fx = Face number x

fyx = Face of a control volume
for a quantity located at F0

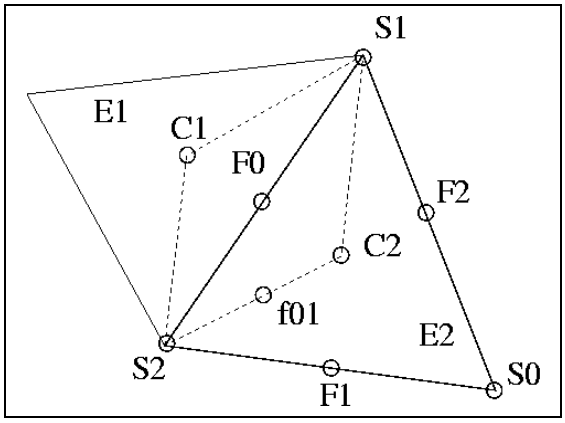


Figure 5.1: Representation of the P1 non conforming discretisation of 2 dimensional control volumes on triangles

The fluxes across the faces of the control volume are calculated depending on the order of the scheme.

a) Monotone Upstream-Centred Scheme for Convective flows (muscl)

To ensure 2nd order accuracy, the flux $uX \cdot S_{fij}$ is estimated as shown for the example of the face f_{01} from the following interpolation formulas:

in 2D : $uX \cdot S_{f01} = (u_{S2} \cdot X_{S2} + u_{C2} \cdot X_{C2} + 4.u_{f01} \cdot X_{f01}) \cdot S_{f01} / 6$

in 3D[7] : $uX \cdot S_{f01} = ((u_{S2}+u_{C2}).(X_{S2}+X_{C2}) + (u_{S2}+u_{S3}).(X_{S2}+X_{S3}) + (u_{C2}+u_{S3}).(X_{C2}+X_{S3})) \cdot S_{f01} / 12$

For all schemes, the transporting quantity (u) is estimated on each point according to the form functions of the P1 non conforming representation. The transported quantity however (u for the momentum equation and T or Y_i for the scalar conservation equation) is estimated from a reconstructed upwind quantity which is dependent on the flow direction:

If $U_{f01}.S_{f01} > 0$:

$X_{S2} = X_{F0} + \text{grad}(X_{F0}) \cdot F_0S_2$;

$X_{f01} = X_{F0} + \text{grad}(X_{F0}) \cdot F_0f_{01}$;

$X_{C2} = 2 \cdot X_{f01} - X_{S2}$

else :

$X_{S2} = X_{F1} + \text{grad}(X_{F1}) \cdot F_1S_2$;

$X_{f01} = X_{F1} + \text{grad}(X_{F1}) \cdot F_1f_{01}$;

$X_{C2} = 2 \cdot X_{f01} - 2 \cdot X_{S2}$

The distances between the locations of F_0 and a second point (S_2 or f_{01}) are abbreviated by F_0S_2 or F_0f_{01}, respectively. Different slope limiters /Ferziger/ are used to calculate $\text{grad}(X_{F0})$, the gradient of the quantity X in the control volume around the face F0 from the gradients of the two associated elements:

$\text{grad}(X_{F0}) = \textit{minmod} (\text{grad}(X_{E1}) ; \text{grad}(X_{E2}))$

or $\text{grad}(X_{F0}) = \textit{Van\_Leer} (\text{grad}(X_{E1}) ; \text{grad}(X_{E2}))$

or $\text{grad}(X_{F0}) = \textit{Van\_Albada} (\text{grad}(X_{E1}) ; \text{grad}(X_{E2}))$

if ($\text{grad}(X_{E1}) \cdot \text{grad}(X_{E2}) < 0$)

minmod ($\text{grad}(X_{E1})$; $\text{grad}(X_{E2})$) = 0

Van_Leer ($\text{grad}(X_{E1})$; $\text{grad}(X_{E2})$) = 0

Van_Albada ($\text{grad}(X_{E1})$; $\text{grad}(X_{E2})$) = 0

else

minmod ($\text{grad}(X_{E1})$; $\text{grad}(X_{E2})$) = $\text{sgn}(\text{grad}(X_{E1})) \cdot \min (| \text{grad}(X_{E1}) | , | \text{grad}(X_{E2}) |)$

Van_Leer ($\text{grad}(X_{E1})$; $\text{grad}(X_{E2})$) = $2 \cdot \text{grad}(X_{E1}) \cdot \text{grad}(X_{E2}) / (\text{grad}(X_{E1}) + \text{grad}(X_{E2}))$

Van_Albada

[7] S_3 denotes in the 3 dimensional case the third vertex associated to the f_{01} face of a tetrahedron

$$(\text{grad}(X_{E1}) ; \text{grad}(X_{E2})) = \text{grad}(X_{E1}) . \text{grad}(X_{E2}) \cdot (\text{grad}(X_{E1}) + \text{grad}(X_{E2})) / (\text{grad}(X_{E1}) \cdot \text{grad}(X_{E1}) + \text{grad}(X_{E2}) \cdot \text{grad}(X_{E2}))$$

b) Upwind (amont)

In accordance to Figure 5.1, for the 1st order upwind scheme, the flux $uX \cdot S_{fij}$ is estimated as shown for the example of the face f_{01} by:

$$uX.S_{f01} = u_{f01} \cdot X_{f01} \cdot S_{f01}$$

The former TVD scheme degenerates to a 1st order upwind scheme by assuming that

$$\text{grad}(X_{F0}) = 0.$$

This assumption leads to the following estimation of the transported quantity:

if ($(U_{f01} \cdot S_{f01}) > 0$)

$X_{f01} = X_{F0}$;

else

$X_{f01} = X_{F1}$.

5.3.1.2 Finite element formulation

a) Centred Scheme (EF)

The convection term is modelled with the EF scheme by a 2nd order centred Finite Element formulation which conserves the kinetic energy. According to the variationnal formulation, the convective term is expressed as $(u\nabla u, v)$ where u designates the P1 non conforming velocity flow field and ν the corresponding reference test functions. Recalling that the gradient is constant in the element,

$$\left(\nabla u_j\right)_i = U_{ji} = \int_{\Omega} \left(\nabla u_j\right)_i dV = \sum_{faces=k} u_j^k \cdot \int_{\Omega} \nabla \Psi_j^k dV = \sum_{faces=k} u_j^k \cdot (-d) \cdot \int_{\Omega} \left(\nabla \lambda_j^k\right)_i dV = \sum_{faces=k} u_j^k S_i^k$$

the convective term is calculated as:

$$(u\nabla u, v)_j^f = \left(U_i U_{ji} V_j\right)^f = \int_{\Omega} u_i^f \Psi^f \cdot \sum_{faces=k} u_j^k S_i^k \cdot \sum_{faces=l} \Psi^l dV = \frac{V}{d+1} u_i^f \sum_{faces=k} u_j^k S_i^k$$

Here, Einstein's convention on subscripts is used. Subscripts refer to the components and exponents to the faces. To ensure kinetic energy conservation, the anti-symmetric part has to be associated to the convective term expression. Since

$$\left((u\nabla u), v\right)_j = \left(U_i U_{ji} V_j\right) = \left[U_i U_j V_j\right]_{\omega} - \left(U_j \left(U_i V_j\right)_i\right) = -\left(U_j U_i V_{ji}\right) = -\left(U_i V_{ji} U_j\right) = -\left((u\nabla v), u\right)_j$$

is true for any domain with periodic or wall boundaries and assuming incompressibility, the convective term is equivalent to:

$$((u\nabla u),v)=\frac{1}{2}[((u\nabla u),v)-((u\nabla v),u)]$$

where

$$(u\nabla v,u)_j^f=\left(U_i V_{ji} U_j\right)^f=\int_\Omega u_i^f \Psi^f \cdot \sum_{faces=k} S_i^k \cdot \sum_{faces=l} u_j^l \Psi^l dV=\frac{V}{d+1} u_i^f u_j^f \sum_{faces=k} S_i^k .$$

It is important to note that the convective term is finally calculated from the P1 velocity flow field. This field is obtained by changing in the previous expression u_i^f to u_j^f. The contribution is projected on a P1 base (vertices) by using the filtering operator:

$$((u\nabla u),v)=\overline{(u\nabla u)}\,.$$

For the transportation of a scalar (T), the previous terms become:

$$(u\nabla T,v)_j^f=\left(U_i T V_j\right)^f=\int_\Omega u_i^f \Psi^f \cdot \sum_{faces=k} T^k S_i^k \cdot \sum_{faces=l} \Psi^l dV=\frac{V}{d+1} u_i^f \sum_{faces=k} T^k S_i^k$$

$$(u\nabla v,T)_j^f=\left(U_i V_{ji} T\right)^f=\int_\Omega u_i^f \Psi^f \cdot \sum_{faces=k} S_i^k \cdot \sum_{faces=l} T^l \Psi^l dV=\frac{V}{d+1} u_i^f T^f \sum_{faces=k} S_i^k$$

b) Total Variation Diminishing Scheme (EF_stab)
For the TVD scheme EF_stab, for the time being, the reader should refer to /Turek/ for details of the scheme. In this convection scheme a limiter is integrated which assures that the transported quantity stays within its physical bounds.

5.3.2 Diffusion term

The diffusion term is discussed here on the example of viscous fluxes. Energy and tracer species diffusive fluxes are treated analogously. This term is discretized by a conservative 2nd order central scheme which is based on the finite volume approach /Emonot/. When using the non specific keyword “diffusion { }” the following terms are treated:

- For isothermal laminar flow as well as for laminar flow with temperature dependent viscosity:

  $\tau^0=\nu\cdot\nabla u$

- For turbulent flow[8]:

[8] The velocities can be mean values (RANS) or filtered values (LES)

$$\tau^0 = \nu \cdot \nabla \bar{u} + \nu_t \left(\nabla \bar{u} + \nabla^T \bar{u} \right)$$

The same formulations are used for the explicit time schemes, the semi implicit time scheme as well as for the Crank Nicholson implicit time scheme which is based on the iterative Jacobi method.

5.3.3 Gravitational acceleration

For incompressible flows, the effect of the gravitational acceleration of a non isothermal, multi component mixture of trace species is treated with Boussinesq approximation:

$$\left(\beta_T \cdot (T - T_0) + \sum_k \beta_{Y,k} \cdot (Y_k - Y_{k,0})\right) \cdot g$$

T_0 is the coldest temperature in a whole transient. β_T is usually calculated for a mean temperature.$Y_{k,0}$ is the lowest concentration of component k in a whole transient. β_Y however, is calculated for a mean concentration.

5.3.4 External forces

User defined volume sources for momentum, energy and tracer species.

5.3.5 Pressure gradient

A 1st order gradient operator is used in the SOLA projection method

$$\nabla P^0$$

This term can not be modified by the user!

5.3.6 Mass conservation

A 1st order divergence operator is used in the SOLA projection method

$$\nabla . u = 0$$

This term can not be modified by the user!

6 Adaptation of the algorithm for quasi-compressible flows

The main elements given in the previous section about the spatial and temporal discretization are always correct for quasi-compressible flows, however we can note a few modifications for the general algorithm.

Mainly, the solving sequence of the equations differs from the incompressible case. The algorithm to compute all the quantities at the time "n+1" from the values at the instant "n" can be quickly written :

1) Computation of all the scalar quantities (T^{n+1}, Y_i^{n+1}) by applying the chosen time scheme

2) Calculation of the thermodynamic pressure P_{th} (constant value or from mass conservation ODE)

3) Update of the density ρ^{n+1} thanks to the equation of state

4) Calculation of u^{n+1} and P_h^{n+1} by combining the continuity equation and the momentum conservation equations (thanks to a similar method to SOLA projection described previously but taking into account the fact $\frac{\rho^{n+1}-\rho^n}{\Delta t} \neq 0$)

7 Recommended modelling of thermal hydraulic problems

We recommend respecting as far as possible the recommendations given in "Best Practice Guidelines" for the use of CFD calculations /OCDE/NEA/. In terms of the keywords, the reader is recommended to refer to the Trio_U user manual.

7.1 Numerical nuclear reactor with MILES modelling

7.1.1 Characterisation of the model

- Extended geometry with geometrically complex internal structures
- Thermal effects are present
- Under-resolved LES turbulence modelling (MILES)
- 2nd order TVD convection scheme (EF_Stab)
- Semi implicit 1st order time discretisation in order to treat the diffusion term implicitly
    - Activation the semi implicit solver with the keyword "diffusion_implicite"

- Ensure that the solver for the implicitly treatment of the diffusion is iterating at least 2 times
    - Adaptation of the convergence criteria with the keyword "seuil_diffusion_implicite"

7.1.2 Initial and boundary conditions

7.1.2.1 Initial conditions

Momentum equation:
Stagnant fluid in whole domain (u=0)
Energy equation:
Constant temperature in whole domain (T=To)
Tracer transport equation:
Constant concentration in whole domain (Y=0)

7.1.2.2 Inflow boundary condition

Momentum equation:
Velocity profile which is constant in space and time
Energy equation:
Temperature profile which is constant in space and time
Tracer transport equation:
Concentration profile which is constant in space and time

7.1.2.3 Outflow boundary condition

Momentum equation:
Constant pressure which is also constant in time (P/ρ_0-gz = 0)
Energy equation:
Diffusive fluxes are zero (invariant in time)
Tracer transport equation:
Diffusive fluxes are zero (invariant in time)

7.1.2.4 Wall boundary condition

Momentum equation:
Logarithmic wall function are applied to all walls
Energy equation:
Adiabatic walls are applied to all walls (heat flux is set to zero)
Tracer transport equation:
Impermeable walls are applied to all walls (mass flux is set to zero)

7.1.3 Turbulence modelling

- Smagorinsky sub-grid model with default values
- Limitation of the maximum of the turbulent viscosity in order to avoid small time steps during the beginning of the transient calculation.
    - Limitation of the maximum of the turbulent viscosity with the keyword “nut_max”

7.1.4 Meshing

- Homogeneous tetra meshing without large variations in the tetra size.
- Delaunay criteria should be respected if possible.
- Mesh refinement near walls in order to respect the application criteria of logarithmic wall functions.
- Minimum 5 better 10 calculation points in gaps between two walls.
- Length scale of the CAD file for ICEM meshing in “mm” and length scale for the Trio_U calculation in “m”.
    - Adaptation of the length scale with the keyword “dilate”
- Correct corner meshing without stand alone vertices (see Figure 5.1).
    - Test and correction of the corner meshing with the keyword “VerifierCoin”

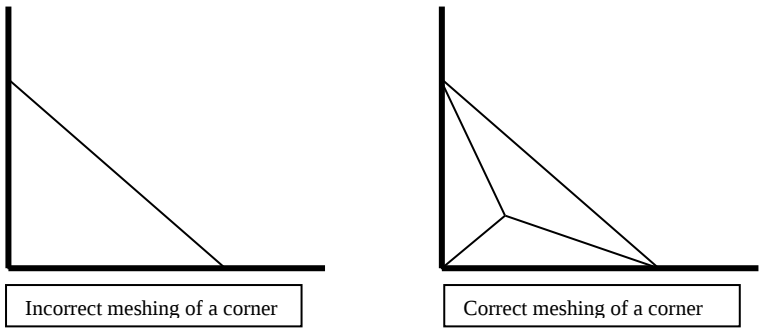


Figure 6.1: Correct meshing of a corner by using the keyword “VerifierCoin”

7.1.5 Trio_U input file

```
# Reactor Calculation with MILES modelling #

# Definition of the dimension #
dimension 3

# Definition of the problem #
Pb_Thermohydraulique_Concentration_Turbulent_Scalaires_Passifs pb

# Definition of the calculation Domain #
Domaine DOM_DOM

# In parallel calculations, the following instructions have to be placed #
# into the input file of the CUTTER #

# Lire_fichier DOM_DOM  trio_DOM_geo.asc #

# dilate DOM_DOM 0.001 #
# VerifierCoins DOM_DOM #

# Read of the Zones of the decomposited domain #
Scatter DOM_44_bin.Zones DOM_DOM

# Definition of the discretisation #
VEFPreP1B dis

# Definition of the time scheme #
Schema_Euler_explicite sch
Lire sch
        {
            tinit 0.0
            tmax 180.
            dt_min 1.e-8
            dt_max 0.004
            dt_impr 1.e-12
            dt_sauv 1000.0
            seuil_statio 1.e-9
            diffusion_implicite 1
            seuil_diffusion_implicite 1.e-7
            facsec 1
            nb_pas_dt_max 30000
        }

# Definition of the fluid properties #
Fluide_Incompressible fluide

# Water at 250°C and 50 bar #
Lire fluide
{
   mu      Champ_Uniforme 1 0.000106
   lambda  Champ_Uniforme 1 0.617
   Cp      Champ_Uniforme 1 4847.
   rho     Champ_Uniforme 1 799.
```

```
   beta_th Champ_Uniforme 1 0.001824
   beta_co Champ_Uniforme 1 0.
}

# Definition of the diffusivity of the tracer #
Constituant c1
Lire c1
{
   diffusivite Champ_Uniforme 1 2.147E-7
}

# Definition of the gravity #
Champ_Uniforme gravite
Lire gravite 3 0. 0. -9.81

# Association of the objects to the problem #
Associer fluide gravite
Associer pb DOM_DOM
Associer pb sch
Associer pb fluide
Associer pb c1

# Discretisation of the problem #
Discretiser pb dis

# Definition of the parameters of the problem #
Lire pb
{
      Navier_Stokes_turbulent
      {
            solveur_pression Gcp
                  { precond ssor { omega 1.5 } seuil 1.e-05 impr }
            convection { EF_stab }
            diffusion { }
            sources { boussinesq_temperature { T0 150. } }
            Modele_turbulence Sous_maille_Smago
                  {
                  Turbulence_paroi loi_standard_hydr
                  nut_max 0.3
                  }
            conditions_initiales
                  {
                  vitesse Champ_Uniforme 3 0. 0. 0.
                  }
            conditions_limites
                  {
                  wall  paroi_fixe
                  in1   frontiere_ouverte_vitesse_imposee
                        Champ_front_uniforme 3  0.  0. 1.
                  in2   frontiere_ouverte_vitesse_imposee
                        Champ_front_uniforme 3  0.  0. 1.
                  in3   frontiere_ouverte_vitesse_imposee
                        Champ_front_uniforme 3  0.  0. 1.
                  out   frontiere_ouverte_pression_imposee
                        Champ_front_Uniforme 1 0.
                  }
```

```
  }
  Convection_Diffusion_Temperature_Turbulent
{
      diffusion { }
      convection { EF_Stab }
      conditions_initiales
            {
            temperature Champ_Uniforme 1 250.
            }
      conditions_limites
      {
                  wall paroi_adiabatique
                  in1  frontiere_ouverte_temperature_imposee
                       Champ_front_Uniforme 1 250.
                   in2  frontiere_ouverte_temperature_imposee
                       Champ_front_Uniforme 1 250.
                   in3  frontiere_ouverte_temperature_imposee
                       Champ_front_Uniforme 1 150.
                  out  frontiere_ouverte T_ext
                       Champ_front_Uniforme 1 250.

      }
      Modele_turbulence Prandtl
            {
               Turbulence_paroi loi_standard_hydr_scalaire
            }
}

  Convection_Diffusion_Concentration_Turbulent
{
          diffusion { }
          convection { EF_Stab }
          conditions_limites
      {
            wall paroi
                  in1  frontiere_ouverte_concentration_imposee
                       Champ_front_Uniforme 1 1
                  in2  frontiere_ouverte_concentration_imposee
                       Champ_front_Uniforme 1 0.
                  in3  frontiere_ouverte_concentration_imposee
                       Champ_front_Uniforme 1 0.
                  out  frontiere_ouverte C_ext
                       Champ_front_Uniforme 1 0.

          }
          conditions_initiales
      {
                   concentration Champ_Uniforme 1 0.
          }
      Modele_turbulence Prandtl
            {
               Turbulence_paroi loi_standard_hydr_scalaire
            }
  }
Equations_Scalaires_Passifs
```

```
    {
          Convection_diffusion_Concentration_Turbulent
       {
                diffusion { }
                convection { EF_Stab }
                conditions_limites
                {
                wall paroi
                in1  frontiere_ouverte_concentration_imposee
                     Champ_front_Uniforme 1 0.
                in2  frontiere_ouverte_concentration_imposee
                     Champ_front_Uniforme 1 1.
                in3  frontiere_ouverte_concentration_imposee
                     Champ_front_Uniforme 1 0.
                out  frontiere_ouverte C_ext
                     Champ_front_Uniforme 1 0.
                }

                conditions_initiales
                {
                        concentration0 Champ_Uniforme 1 0.
                }
                Modele_turbulence Prandtl
                {
                   Turbulence_paroi loi_standard_hydr_scalaire
                }
          }

          Convection_diffusion_Concentration_Turbulent
       {
                diffusion { }
                convection { EF_Stab }
                conditions_limites
                {
                wall paroi
                in1  frontiere_ouverte_concentration_imposee
                     Champ_front_Uniforme 1 0.
                in2  frontiere_ouverte_concentration_imposee
                     Champ_front_Uniforme 1 0.
                in3  frontiere_ouverte_concentration_imposee
                     Champ_front_Uniforme 1 1.
                out  frontiere_ouverte C_ext
                     Champ_front_Uniforme 1 0.
                }

                conditions_initiales
                {
                   concentration1 Champ_Uniforme 1 0.
                }
                Modele_turbulence Prandtl
                {
                   Turbulence_paroi loi_standard_hydr_scalaire
                }
          }
    }
Postraitements
```

```
        {
             first_post
                  {
                    fichier Post_meshtv
                    format meshtv
                 Sondes
                 {
                       pres_point pression periode 0.0001 points
                             1     0.      0.     -1.220
                 }
                     Champs dt_post 1.0
                 {
                       temperature elem
                      concentration elem
                      concentration0 elem
                      concentration1 elem
                      vitesse
                      Y_plus elem
                      viscosite_turbulente elem
                  }
                  }
                 second_post
                     {
                     fichier Post_lata
                     Format lata
                     Champs Binaire dt_post 0.25
                        {
                             temperature elem
                             vitesse
                             concentration elem
                             concentration0 elem
                             concentration1 elem
                        }
                     }
          }
}

EcritureLectureSpecial 1

Resoudre pb
Fin
```

7.2 Turbulent flow with RANS modelling

7.2.1 Characterisation of the model

- Tube geometry with sudden expansion
- Azimuthally not the whole tube (360°) is treated but only a slice of 30°
- RANS turbulence modelling (k-ε)
- Fully explicit time scheme
- 2nd order TVD convection schemes for both momentum and k-ε transport (EF_Stab) (amont is recommended for fully implicit calculations)

7.2.2 Initial and boundary conditions

7.2.2.1 Initial conditions

Momentum equation:
Stagnant fluid in whole domain (u=0)
k-ε transport equation:
Constant values in whole domain

7.2.2.2 Inflow boundary condition

Momentum equation:
Velocity profile which is constant in space and time
k-ε transport equation:
Profiles which are constant in space and time

7.2.2.3 Outflow boundary condition

Momentum equation:
Constant pressure which is also constant in time (P/ρ_0-gz = 0)
k-ε transport equation:
Diffusive fluxes are zero (invariant in time)

7.2.2.4 Wall boundary condition

Momentum equation:
Logarithmic wall function are applied to all walls
k-ε transport equation:
Wall function for fully developed turbulent flow are used

7.2.3 Turbulence modelling

- k-ε model with default coefficients

7.2.4 Meshing

- Homogeneous tetra meshing without large variations in the tetra size.
- Delaunay criteria should be respected if possible.
- Mesh refinement near walls in order to respect the application criteria of logarithmic wall functions.
- Minimum 5 better 10 calculation points in gaps between two walls.
- Length scale of the CAD file for ICEM meshing in “mm” and length scale for the Trio_U calculation in “m”.
    - Adaptation of the length scale with the keyword “dilate”
- Correct corner meshing without stand alone vertices (see Figure 5.1).
    - Test and correction of the corner meshing with the keyword “VerifierCoin”

7.2.5 Trio_U input file

```
# Expanding tube calculation with RANS modelling #

# Definition of the dimension #
dimension 3

# Definition of the problem #
Pb_Hydraulique_Turbulent pb

# Definition of the calculation Domain #
Domaine DOM_DOM

# Read of the meshing #
Lire_fichier DOM_DOM trio_DOM_geo.asc

#Correction of the mesh #
Dilate DOM_DOM 0.001
VerifierCoin DOM_DOM

# Definition of the discretisation #
VEFPreP1B dis

# Definition of the time scheme #
schema_Euler_explicite sch
Lire sch
{
      tinit 0.00
      tmax 32.0
      dt_min 1.e-8
      dt_max 0.1
      dt_impr 5.e-2
      dt_sauv 1000.
      seuil_statio 1.e-8
}

# Definition of the fluid properties #
Fluide_Incompressible fluide

# Water at 20°C and 1 bar #
Lire fluide
{
      mu  Champ_Uniforme 1 1.121e-7
      rho Champ_Uniforme 1 1.0
}

# Association of the objects to the problem #
Associer pb DOM_DOM
Associer pb sch
Associer pb fluide

Discretiser pb dis

# Definition of the parameters of the problem #
```

```
Lire pb
{
      Navier_Stokes_Turbulent
      {
            solveur_pression GCP { precond ssor { omega 1.5O }
                  seuil 1.Oe-O6 }
            convection { EF_stab }
            diffusion { }
            conditions_initiales {
                  vitesse Champ_Uniforme 3  O. O. O.
                  }
            conditions_limites {
                   WALL  Paroi_Fixe
                   SYM   Symetrie
                   IN    frontiere_ouverte_vitesse_imposee
                         Champ_Front_Uniforme 3  O. 1. O.
                   OUT   frontiere_ouverte_pression_imposee
                         Champ_Front_Uniforme 1  O.
                   }
            Modele_turbulence K_Epsilon
            {
             Transport_K_Epsilon
             {
             convection  { EF_stab }
             diffusion { }
             conditions_initiales
                   {
                    k_eps Champ_Uniforme 2  5.e-3  1.e-5
                  }
            conditions_limites
            {
                   WALL  Paroi
                   SYM   Symetrie
                   IN    frontiere_ouverte_k_eps_impose
                         Champ_Front_Uniforme 2 5.e-3  1.e-4
                   OUT   frontiere_ouverte k_eps_ext
                         Champ_Front_Uniforme 2 1.e-3  1.e-4
                   }
                      }
            turbulence_paroi loi_standard_hydr dt_impr_ustar 1.
           }
      }
      Postraitement
      {
            Sondes
            {
                  sonde_vitesse1  vitesseY  periode 2.0
                        Segment 5O   0.0  0.0  0.0   0.0   3.0  0.0
            }
            format meshtv Champs dt_post 2O.
            {
                  pression elem
                  vitesse elem
                  k  elem
                  eps elem
                  y_plus elem
```

```
                    viscosite_turbulente elem
                }
            }

        }
EcritureLectureSpecial 0
Resoudre pb
Fin
```

7.3 Turbulent flow with fine LES modelling

7.3.1 Characterisation of the model

- Tube like geometry
- Azimuthally the whole test section is treated
- Thermal effects are not present (the temperature act as a tracer)
- The inflow is highly turbulent
- Resolved LES turbulence modelling
- Turbulent fluctuations imposed at one inlet
- Implicit time scheme (Crank-Nicholson)
- 2^{nd} order centred convection schemes for the momentum equation (EF)
- 2^{nd} order TVD convection schemes for the scalars (EF_Stab)

7.3.2 Initial and boundary conditions

7.3.2.1 Initial conditions

Momentum equation:
Stagnant fluid in whole domain (u=0)
Energy equation:
Constant temperature in whole domain (T=242°C)

7.3.2.2 Inflow boundary condition

Momentum equation:

1. Velocity profile which is constant in space and time
2. Constant velocity profile with superimposed turbulent fluctuations

Energy equation:
Temperature profile which is constant in space and time

7.3.2.3 Outflow boundary condition

Momentum equation:
Constant pressure which is also constant in time (P/ρ_0-gz = 0)
Energy equation:
Diffusive fluxes are zero (invariant in time)

7.3.2.4 Wall boundary condition

Momentum equation:
Logarithmic wall function are applied to all walls
Energy equation:

1. Adiabatic walls are applied (heat flux is set to zero)

2. Walls with an imposed hest flux distribution are applied

7.3.3 Turbulence modelling

- WALE sub-grid model with default values

7.3.4 Volume sources

- A volume energy source is defined in order to take into account the decay heat released in the fluid. The source is variable in space but constant in time.

7.3.5 Meshing

- Homogeneous tetra meshing without large variations in the tetra size.
- Delaunay criteria should be respected if possible.
- Mesh refinement near walls in order to respect the application criteria of logarithmic wall functions.
- Minimum 5 better 10 calculation points in gaps between two walls.

7.3.6 Trio_U input file

```
# Fine LES Simulation #

# Definition of the dimension #
dimension 3

# Definition of the problem #
Pb_ThermoHydraulique_Turbulent pb

# Definition of the calculation Domains #
# 1st domain = TEST domain #
# 2nd domain = Recirculation box for turbulent fluctuation creation #
Domaine dom_TEST
Domaine dom_BOXDC

# Read of the Zones of the decomposited domain #
Scatter TEST.Zones dom_TEST
Scatter BOXDC.Zones dom_BOXDC

# Definition of the discretisation #
VEFPreP1B dis

# Definition of the time scheme #
Schema_CN_EX_iteratif sch
Lire sch
{
        dt_start dt_fixe 7.99e-05
        tinit 3.050007
        tmax  3.10
        dt_min 1.e-7
        dt_max 1.e-1
        dt_impr 0.0125
        dt_sauv 1000.
        seuil_statio 1.e-8
}

# Definition of the fluid properties #
Fluide_Incompressible fluide

# Fluid properties: Eutectic mixture of Pb/Bi at 240°C #
Lire fluide
{
        mu        Champ_Uniforme    1 0.002
        rho       Champ_Uniforme    1 10400.
        lambda    Champ_Uniforme    1 10.09
        Cp        Champ_Uniforme    1 146.5
}


# Association of the objects to the problem #
Associer pb     dom_TEST
Associer pb     fluide

Pb_Hydraulique_Turbulent pb_BOXDC
Associer pb_BOXDC dom_BOXDC
```

```
Associer pb_BOXDC fluide

Probleme_Couple pbc
Associer pbc    pb_BOXDC
Associer pbc    pb
Associer pbc    sch
Discretiser pbc dis

Lire pb
{
        Navier_Stokes_turbulent
        {
            dt_projection 0.025 1.e-8
       solveur_pression Gcp { precond ssor { omega 1.5 } seuil 1.e-06
impr }
       solveur_bar      Gcp { precond ssor { omega 1.5 } seuil 1.e-10 }
       convection { EF  defaut_bar }
       diffusion  { standard  defaut_bar }
       Sources { Source_Qdm_lambdaup  2. }
                conditions_initiales { vitesse champ_Uniforme 3 0. 0. 0. }
                conditions_limites {
                        INLDC Frontiere_ouverte_vitesse_imposee
                        Champ_front_calc_recycl_fluct_pbperio
                              pb_BOXDC PERIO  pb INLDC vitesse 3 3 1. -1.
                        INLBP frontiere_ouverte_vitesse_imposee
                              champ_front_fonc_xyz 3 0. 0. -0.343*6*
(SQRT(Y*Y)-0.065)*(0.085-SQRT(Y*Y))/0.0004
                       OUTLE frontiere_ouverte_pression_imposee
                       champ_front_uniforme 1 0.
                       WALLS paroi_fixe
                       WWINT paroi_fixe
                       }
                modele_turbulence sous_maille_wale
                  {
                        turbulence_paroi loi_standard_hydr
                  }
      }
        Convection_Diffusion_Temperature_turbulent
        {
                convection { EF_stab }
                diffusion { }
                sources { Puissance_Thermique champ_fonc_xyz dom_TEST 1
                        (Z<0.27)*1.48E+9*EXP(-(Z-0.088+SQRT(0.088^2-
(X^2+Y^2)))/0.145)*(1.0-EXP(-(Z-0.088+SQRT(0.088^2-
(X^2+Y^2))+0.045)/0.045))*(1.0+550.*(0.267-(Z-0.088+SQRT(0.088^2-
(X^2+Y^2))))*EXP(-SQRT((0.267-(Z-0.088+SQRT(0.088^2-
(X^2+Y^2))))^2)/0.0045))*EXP(-
0.5*((X/(0.0205+0.0155*Z+0.121*Z*Z))^2+(Y/(0.0256+0.0256*Z+0.0839*Z*Z))^2))
                  }
                conditions_initiales { Temperature champ_Uniforme 1 242. }
                conditions_limites
                        {
                        INLDC frontiere_ouverte_temperature_imposee
                              champ_front_uniforme 1 242.
                        INLBP frontiere_ouverte_temperature_imposee
                              champ_front_uniforme 1 242.
```

```
                        OUTLE frontiere_ouverte T_ext
                              champ_front_uniforme 1 242.
                        WALLS paroi_adiabatique
                        WWINT paroi_flux_impose champ_front_fonc_xyz 1
0.0016*1.428E+9*EXP(-0.5*((X/0.021)^2+(Y/0.0378)^2))
                        }
                Modele_turbulence Prandtl
                {
                        Turbulence_paroi negligeable_scalaire
                }
      }
        Postraitement
        {
        format meshtv
            Sondes
                {
                   VITES vitesse periode 0.001 point  3 0. -0.062  0.047
                                                         0. -0.060  0.049
                                                         0. -0.055  0.061
                }
                Champs dt_post 1.e-2
                {
            vitesse som
            temperature som
                }
      }
      reprise formatte Sauv/TEST3.05.sauv
      sauvegarde formatte Sauv/TEST3.10.sauv
}

Lire pb_BOXDC
{
 Navier_Stokes_Turbulent
 {
       solveur_pression Gcp { precond ssor { omega 1.5 }
                                           seuil 1.e-08
                            }
       solveur_bar      Gcp { precond ssor { omega 1.5 }
                                           seuil 1.e-12
                            }
       convection { EF  defaut_bar }
       diffusion  { standard  defaut_bar }
       Sources { Source_Qdm_lambdaup  2. }
       Sources
       {
       Canal_perio { direction_ecoulement 2 }
       }
       conditions_initiales { vitesse Champ_fonc_reprise
                              boxDC_pb.xyz pb_BOXDC vitesse 5.000242 }
       conditions_limites {
                   PERIO    periodique direction_periodicite Z
                   PAROI    paroi_fixe
                          }
        Modele_turbulence Sous_maille_wale
                          {
                          turbulence_paroi loi_standard_hydr
```

```
                dt_impr_ustar 5.
                      }
 }
 Postraitement
      {

           Sondes
            {
            VITEBOX   vitesse periode 0.001   points 1  0. +0.075  0.325
          }
                Champs dt_post 1.e-2
                {
            vitesse som
                }
      }
      reprise formatte ./SauvBox/boxDC.sauv
      sauvegarde formatte ./SauvBox/boxDC_3.1.sauv
}

EcritureLectureSpecial 0
Resoudre pbc
Fin
```

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