CHAPTER – 3

METHODOLOGY

3.1 Introduction

The STAR-CD code is based on the finite volume approach where the computational domain is divided into control volumes by a computational mesh which can dynamically distort to accommodate for moving boundaries like piston and valves. The governing equations\textsuperscript{[69]} for the conservation of mass, momentum, energy, and species concentration for gas and spray droplets, together with an equation of stage, are approximated by algebraic forms for each mesh cell. The resulting set of equation of state, are approximated by algebraic forms for each mesh cell. The resulting set of equations is solved numerically to obtain the gas and spray motions, the fuel evaporation, mixing and combustion. The small-scale turbulence effects are modeled indirectly within the Reynolds averaging framework, using high Reynolds number $k-\varepsilon$ turbulence models with associated wall functions.

3.2 Basic Governing Equations\textsuperscript{[96]}

Continuity:

$$\frac{\partial}{\partial t}(\alpha_i \rho_k) + \nabla \cdot (\alpha_i \rho_k u_i) = 0$$  \hspace{1cm} (3.1)

Where $\alpha_i$ - volume fraction
\( \rho_k \) - density

\( u_k \) - mean phase velocity

In addition, the volume fractions must satisfy \( \sum_{k=1}^{d} \alpha_k = 1 \)

**Momentum:**

\[
\frac{\partial}{\partial t} (\alpha_k \rho_k u_k) + \nabla \cdot (\alpha_k \rho_k u_k u_k) =
- \alpha_k \nabla p + \alpha_k \rho_k g + \nabla \cdot \left[ \alpha_k (\tau_k + \tau_k') + M_k + (F_{\text{int}})_k \right] \tag{3.2}
\]

Where \( \tau_k \) and \( \tau_k' \) - laminar and turbulent stresses, respectively

\( p \) - pressure, assumed to be equal in both phases

\( M_k \) - inter-phase momentum transfer per unit volume

\( (F_{\text{int}})_k \) - internal forces

\( g \) - gravity vector

The inter-phase momentum transfer represents the sum of all the forces the phases exert on one another and satisfies \( M_c = -M_d \).

The internal forces represent forces within a phase. In the current release, they are limited to particle-particle interaction forces in the dispersed phase.

**Energy:**

Energy is solved for static enthalpy in chemico-thermal form.

\[
\frac{\partial}{\partial t} (\alpha_k \rho_k h_k) + \nabla \cdot (\alpha_k \rho_k u_k h_k) - \nabla \cdot \left[ \alpha_k \left( \lambda_k \nabla T_k + \frac{\mu_k}{\sigma_h} \nabla h_k \right) \right] =
- \alpha_k \frac{D_p}{D_t} + \alpha_k (\tau_k + \tau_k') \cdot \nabla u_k + Q_k \tag{3.3}
\]
Where $h_k$ - static enthalpy

$\lambda_k$ - thermal conductivity

$T_k$ - temperature

$\mu'_k$ - turbulent eddy viscosity

$\sigma'_k$ - turbulent thermal diffusion Prandtl number

$Q_k$ - inter-phase heat transfer

**Turbulence:**

Flow turbulence is modeled based on the High Reynolds number $k - \varepsilon$ model. Modified equations are solved for the first phase and the turbulence of the second phase is correlated using semi-empirical models. The additional terms account for the effect of particles on the turbulence field.

\[
\frac{\partial}{\partial t} (\alpha_c \rho_e k_c) + \nabla \cdot (\alpha_c \rho_e \nabla k_c) =
\nabla \cdot \left( \frac{\alpha_c (\mu_e + \mu'_e)}{\sigma_k} \nabla k_c \right) + \alpha_c (G - \rho_e \varepsilon_e) + S_{k2} \tag{3.4}
\]

\[
\frac{\partial}{\partial t} (\alpha_c \rho_e \varepsilon_e) + \nabla \cdot (\alpha_c \rho_e \mu_e \varepsilon_e) =
\nabla \cdot \left( \frac{\alpha_c (\mu_e + \mu'_e)}{\sigma_k} \nabla \varepsilon_e \right) + \alpha_c \frac{\varepsilon_e}{k_c} (C_1 G - C_2 \rho_e \varepsilon_e) + S_{\varepsilon2} \tag{3.5}
\]

Where $k_c$ - continuous phase turbulent kinetic energy

$\mu_e$ - continuous phase molecular viscosity

$\sigma_k$ - turbulent Prandtl number for $k$ equation
\( \varepsilon_c \) - dissipation rate of \( k_c \)

\( \sigma_\varepsilon \) - turbulent Prandtl number for \( \varepsilon \) equation

\( C_1, C_2 \) - constants for High Reynolds number \( k - \varepsilon \) model

\[ G = \mu_e \left[ \nabla u_e + (\nabla u_e)^T \right] \cdot \nabla u_e \]

And the terms \( S_{12} \) and \( S_{e2} \) represent two-phase interactions.

### 3.3 Lagrangian Model (Dispersed Multi-Phase Flow)

In case of the flow consists of a continuous phase, which may be gaseous or liquid, and one or more dispersed phases in the form of liquid droplets or gases bubbles. In general, the motion of the dispersed phase will be influenced by that of the continuous one and vice versa via displacement and inter-phase momentum, mass and heat transfer effects. The strength of the interactions will depend on the dispersed particle’s size, density and number density.

If the flow is laminar, each element released from a point will follow a smooth unique trajectory, i.e. the motion is deterministic. On the other hand, individual elements introduced into a turbulent carrier flow will each have their own, random path due to interaction with the fluctuating turbulent velocity field. Elements may also interact with each other (i.e. collision).

In case of dispersed phase is volatile, soluble or reactive, mass transfer occurs between the phases. This is accompanied by inter-phase heat transfer, which may also arise due to the inter-phase temperature differences. Inter-phase mass transfer causes size
changes in the dispersed elements. Thus, even if the initial size
distribution is uniform, these effects will produce a variable-size
population.

The size change may also be produced by fluid-dynamic forces
acting on the dispersed elements, causing them to break up into
smaller elements. Inter-element collision processes may also produce
the opposite effect, i.e. size increase due to coalescence or
agglomeration.

An additional phenomenon may occur if the dispersed elements
strike a wall. For example, the result may be bouncing or shattering,
according to the impact conditions. STAR-CD provides a dispersed
multi-phase flow modelling framework that is able to encompass all of
the above phenomena. The framework is of Lagrangian/Eulerian
Kind, in which the conservation of mass, momentum and energy for
the dispersed phase.

### 3.3.1 Basic Conservation Equations (Dispersed Phase)

The instantaneous fluid velocity and droplet velocity are denoted
by \('u'\) and \(\dot{u}_d\), respectively. The subscript \(d\) denotes the
droplet/dispersed phase, non-subscripted quantities are taken to refer
to the continuous phase and the droplet position vector is denoted
by \(x_d\). The conservation equations for droplets in the Lagrangian
framework are as follows:
**Momentum:**

The momentum equation for a droplet of mass $m_d$ is

$$m_d \frac{du_d}{dt} = F_{dr} + F_p + F_{am} + F_b$$  \hspace{1cm} (3.6)

Here:

1. $F_{dr}$ is the drag force given by

$$F_{dr} = \frac{1}{2} C_d \rho A_d |u - u_d| (u - u_d)$$  \hspace{1cm} (3.7)

Where $C_d$ is the drag coefficient (a function of the ‘droplet Reynolds number’) and $A_d$ the droplet cross-sectional area.

2. $F_p$ is the pressure force given by

$$F_p = -V_d \nabla p$$  \hspace{1cm} (3.8)

Where $V_d$ is the droplet volume and $\nabla p$ the pressure gradient in the carrier fluid. $p$ includes any hydrostatic components.

3. $F_{am}$ is the so-called ‘virtual mass’ force, i.e. that required to accelerate the carrier fluid ‘entrained’ by the droplet. The expression for this is

$$F_{am} = -C_{am} \rho V_d \frac{d(u_d - u)}{dt}$$  \hspace{1cm} (3.9)

Where $C_{am}$ is the virtual mass coefficient, usually set to 0.5.

Knowledge of the droplet velocity allows its instantaneous position vector $x_d$ to be determined by intergrading:

$$\frac{dx_d}{dt} = u_d$$  \hspace{1cm} (3.10)
From equation (3.3.2), the momentum relaxation time scale $\tau_M$ can be identified as

$$
\tau_M = \frac{m_d |u - u_d|}{F_{de}} = \frac{2m_d}{C_d \rho A_d |u - u_d|} = \frac{4 \rho_d D_d}{3 C_d \rho |u - u_d|}
$$

(3.11)

**Mass:**

In the presence of mass transfer at a rate $F_m$ per unit surface area, the droplet mass rate of change is given by

$$
\frac{dm_d}{dt} = -A_s F_m
$$

(3.12)

Where $A_s$ is the droplet surface area. For an evaporating/condensing single-component droplet, $F_m$ is expressed as [3.3.4]

$$
F_m = K_g p_i \ln \left( \frac{p_t - p_{v,\infty}}{p_t - p_{v,s}} \right)
$$

(3.13)

Where $K_g$ is the mass transfer coefficient and $p_t, p_{v,\infty}$ and $p_{v,s}$ are the gas pressure and partial pressures of the vapour in the droplet surroundings and at its surface, respectively. The surface vapour pressure is assumed to be equal to the saturation pressure at the droplet temperature $T_d$.

From equation [3.12 and 3.13], the mass relaxation time scale $\tau_m$ may be defined as

$$
\tau_m = \frac{m_d}{F_m} = \frac{\rho_d D_d}{6 |F_m|} = \frac{\rho_d D_d}{6 K_g p_i \ln \left( \frac{p_t - p_{v,\infty}}{p_t - p_{v,s}} \right)}
$$

(3.14)
Energy:

The droplet energy balance takes into account the mechanisms of surface heat transfer rates \( q_d^* \) per unit surface area and loss/gain due to phase change, thus:

\[
\frac{m_d}{A} \frac{d}{dt} \left( c_{p,d} T_d \right) = -A_d q_d^* + h_{fg} \frac{dm_d}{dt}
\]

(3.15)

Where \( A_d \) is the droplet surface area, \( c_{p,d} \) the droplet specific heat and \( h_{fg} \) the latent heat of phase change. The surface heat flux, \( q_d^* \), is given by the following relation:

\[
q_d^* = h(T_d - T)
\]

(3.16)

Where \( h \) is the heat transfer coefficient.

From equation (3.15) and 3.16), the thermal relaxation time scale for droplets \( \tau_T \) can be identified as

\[
\tau_T = \frac{c_{p,d} T_d m_d}{A_d q_d} = \frac{c_{p,d} \rho_d D_d}{6h} = \frac{c_{p,d} \rho_d D_d^2}{6K_m Nu}
\]

(3.17)

Where \( K_m \) is the carrier fluid’s conductivity and \( Nu \) the Nusselt number.

3.3.2 Droplet Break-up Models

Droplets may become unstable under the action of the interfacial forces induced by their motion relative to the continuous phase. System-specific models exist for this process and STAR-CD
incorporates a set widely used for the break-up of liquid droplets in a
gaseous stream. The currently available models are:

- Reitz and Diwakar
- Pilch and Erdman
- Hsiang and Faeth

**Reitz and Diwakar model:**

According to this mode, droplet break-up due to aerodynamic
forces occurs in one of the following models:

1. ‘Bag break-up’, in which the non-uniform pressure field around
   the droplet causes it to expand in the low-pressure wake region
   and eventually disintegrate when surface tension forces are
   overcome.

2. ‘Stripping break-up’, a process in which liquid is sheared or
   stripped from the droplet surface.

The break-up rate to be calculated from

\[
\frac{dD_d}{dt} = \frac{(D_d - D_{d,stable})}{\tau_b}
\]  

(3.18)

Where \(D_d\) is the instantaneous droplet diameter. The criteria

time scales are as follows:

**Bag break-up:**

Here, instability is determined by a critical value of the Weber
number, \(We\), thus:

\[
We = \frac{\rho |u - u_d|}{2\sigma_d} \geq C_{bl}
\]  

(3.19)
Where $\sigma_d$ is the surface tension coefficient, and $C_{b1}$ is an empirical coefficient having a value in the range 3.6 to 8.4 [3.3.8]. STAR-CD used $C_{b1}$ = 6 as the default setting. The stable droplet size is that which satisfies the equality in the above equation.

The associated characteristic time is

$$\tau_b = \frac{C_{b2} \rho_d^{1/2} D_d^{3/2}}{4 \sigma_d^{1/2}}$$

(3.20)

In which $C_{b2} \approx \pi$.

**Stripping Break-up:**

The criterion for the onset of this regime is

$$\frac{We}{\sqrt{Re_d}} \geq C_{s1}$$

(3.21)

Where $Re_d$ is the droplet Reynolds number and $C_{s1}$ is a coefficient with the value 0.5.

The characteristic time scale for this regime is

$$\tau_b = \frac{C_{s2}}{2} \left[ \frac{\rho_d}{\rho} \right]^{1/2} \frac{D_d}{\mu - u_d}$$

(3.22)

Here, the empirical coefficient $C_{s2}$ is 20.

### 3.3.3 Inter-Droplet Collisions

A cell clustering mechanism that allows parcels in neighboring cells to collide. Two prerequisites must be met if two parcels are to collide. The first is that they must be traveling towards each other.
The second condition that must be satisfied is that the parcels’ relative displacement must be larger than the distance between them. If these two requirements are met, the parcels have a chance of colliding.

The collision distinguishes between the following three types of interactions:

- Coalescence
- Separation
- Bouncing

When separation or bouncing occurs, only momentum is exchanged between droplets in coalescence mass and energy also exchanged. In modeling these processes, a statistical rather than a deterministic approach is used to avoid creating an excessive number of new parcels.

The droplets are considered to be uniformly distributed throughout the cell, so that the collision frequency, \( v \), of a collector droplet with all droplet with all droplets in the other parcel is given by

\[
v = \frac{\pi}{4} \left( D_{d,1} + D_{d,2} \right)^2 \left| u_{d,1} - u_{d,2} \right| E_{1,2} \frac{N_{d,2}}{\delta V}
\]

Here the subscripts 1 and 2 refer to the collector and donor parcels, respectively, \( N_{d,2} \) is the number of droplets in the second parcel, and \( \delta V \) is the cell volume.

The collision efficiency, \( E_{1,2} \), is evaluated form

\[
E_{1,2} = \left( 1 + \frac{0.75 \ln(2W)}{W - 1.214} \right)^{-2} \quad W \geq 1.214
\]
Otherwise $E_{i,2} = 0$. In this equation, $W$ is a dimensionless parameter given by

$$W = \frac{\rho_d u_d - u_d^2}{9 \mu D_{d,1}}$$

(3.25)

The probability that the collector undergoes $n$ collisions with droplets from a donor parcel during the time interval $\delta t$ is taken to follow a Poisson distribution with a mean value $n' = \nu \delta t$, i.e.

$$P_n = \left( \frac{n'}{n!} \right) e^{-n'}$$

(3.26)

The case $n' = 0$ gives probability of no collision, $P_0 = e^{-n'}$. To determine whether collision take place between individual droplets, a random number $N_{r,1}$ is chosen in the interval (0-1). If $N_{r,1} < P_0$, no collision occurs.

If a collision occurs, the probability that the outcome is coalescence of the droplets is given by:

$$E_{cool} = \min \left[ \frac{2.4 f(\gamma)}{W_{el}} \right]$$

(3.27)

Where $f(\gamma)$ is the function $f(\gamma) = \gamma^3 - 2.4 \gamma + 2.7$, $\gamma = \frac{D_{d,1}}{D_{d,2}}$, and $W_{el}$ is the droplet Weber number defined as

$$W_{el} = \frac{\rho_d u_d - u_d^2}{2 \sigma}$$

(3.28)

To determine whether an individual collision results in coalescence or separation, a second random number $N_{r,2} < E_{cool}$, coalescence occurs
and the number of droplets \( m \) which take part in the coalescence with each collector droplet is

\[
\sum_{i=0}^{i=m-1} \frac{P_i}{P_0} < \frac{N_{r,i}}{P_0} < \sum_{i=0}^{i=m} \frac{P_i}{P_0}
\]  

(3.29)

Thus, the new number of droplets in the donor parcel is \( n_{d,2}^n = N_{d,2} - mN_{d,1} \). The properties of the collector droplets are recomputed so that mass, momentum and energy are conserved. In the case when the condition \( N_{r,2} < E_{coal} \) and the additional requirement \( We_k < We_{bou} \) are satisfied, another type of collision called ‘bouncing’ occurs, where \( We_{bou} \) is obtained from:

\[
We_{bou} = 2.4f(y)N_{r,2}^3
\]  

(3.30)

When separation or bouncing occurs, only momentum is exchanged (and conserved overall).

**3.3.4 Boiling Model**

The model covers those situations when the droplet temperature reaches the boiling or critical temperature. The following conditions are considered:

1. \( T_d > T_c \)

   Here, \( T_c \) is the critical temperature, i.e. the temperature at which \( \left( \frac{\partial p}{\partial V} \right)_{T_c} = 0 \)

2. \( T_d \geq T_b(p_t) \)
Here, $T_b$ is the boiling temperature at the ambient pressure. The boiling temperature is defined by the temperature at which the pressure of saturation, $p_s$, balances the gas pressure, i.e.

$$p_s(T_b) = p_t$$

Note that the user must supply $p_s(T_d) \geq p_t$.

**Mass transfer:**

If condition 1 is satisfied, then the droplet evaporates instantaneously. If condition 2 is satisfied, then the rate of mass transfer, $\frac{dm_d}{dt}$, is given by:

$$\frac{dm_d}{dt} = -2\pi \frac{k}{c_p} D_d \left(1 + 0.23 \text{Re}^{1/2}\right) \ln \left[1 + \frac{c_p (T - T_d)}{h_{fg}}\right]$$

(3.31)

Where $k$ is the conductivity and $c_p$ the specific heat of the mixture.

**Heat transfer:**

During boiling $T_d$ remains constant. Therefore, the rate of heat transfer from carrier fluid to droplet is given by:

$$q_g = -h_{fg} \frac{dm_d}{dt}$$

(3.32)

### 3.4 Inlet Fuel Flow Model

#### 3.4.1 Introduction

The injection process being modeled includes the flow in the nozzle hole and atomization. The latter gives rise to a fuel droplet
spray represented by a set of computational parcels, each containing a number of droplets with the same properties. These properties are calculated on the basis of various atomization models. The histories of the computational parcels are obtained from the Lagrangian conservation equations of mass, momentum and energy.

**Nozzle flow model:**

The injection velocity, $u_{ch}$, i.e. the velocity of the liquid fuel as it exits the nozzle and enters the combustion chamber, is one of the most important parameter in a spray calculation. It strongly influences the atomization and break-up processes, the spray penetration, the inter-phase transfer processes and also the droplet-droplet and droplet-wall interactions.

An 'effective nozzle' model is available in STAR-CD, requiring the nozzle hole diameter, $D$, as a parameter.

### 3.4.2 Atomisation models

The following two atomisation models are supported:

1. Huh’s atomisation model
2. Reitz-Diwakar model

**Huh’s atomisation model**

Huh’s model is based on the premise, supported by order-of-magnitude estimates, that the two most important mechanisms in spray atomisation are the gas inertia and the internal turbulence
stresses generated in the nozzle. A conceptual picture can be described in two stages:

1. The turbulence generated in the nozzle hole produces initial perturbations on the jet surface when it exits the hole.
2. Once the perturbations have reached a certain level, they grow exponentially via pressure forces induced through interaction with the surrounding gas (surface wave growth), until these perturbations become detached from the jet surface as droplets.

The model estimates the initial perturbations from an analysis of the flow through the hole and then uses established wave growth theory, derived from force and energy balances:

\[
k_a = \frac{U^2}{8L} \left( \frac{1}{c_d^2} - K_c - 1 \right) \tag{3.33}
\]

\[
\varepsilon_a = \frac{K_c U^{1/3}}{2L} \left( \frac{1}{c_d^2} - K_c - 1 \right) \tag{3.34}
\]

Where \( U \) is the average injection velocity over the time period of injection, \( L \) and \( K_c \) are the whole length and from loss coefficient, respectively, \( K_c \) is an empirical coefficient and \( c_d \) is the nozzle’s discharge coefficient. \( K_c \) and \( K_c \) are given in table 3-1.

The corresponding turbulence length and time scale are:

\[
L_i^0 = C_\mu \frac{k_a^{5/4}}{\varepsilon_a} \tag{3.35}
\]

\[
\tau_i^0 = C_\mu \frac{k_a}{\varepsilon_a} \tag{3.36}
\]
Where $C_\mu$ is the coefficient of the $k-\varepsilon$ model. Each injected (parent) droplet is assigned these as the initial values. Thereafter the turbulence within it decays with time, and the following relations describe this time dependence:

$$L_i(t) = L_i^0 \left(1 + C_{a1} \frac{t}{\tau_i^0}\right)^{C_{a2}} \tag{3.37}$$

$$\tau_i(t) = \tau_i^0 \left(1 + C_{a1} \frac{t}{\tau_i^0}\right) \tag{3.38}$$

Where $C_{a1}$ and $C_{a2}$ are the model coefficients, given in table 3-1

<table>
<thead>
<tr>
<th>$C_\mu$</th>
<th>$K_c$</th>
<th>$K_x$</th>
<th>$C_{a1}$</th>
<th>$C_{a2}$</th>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
<th>$C_4$</th>
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<td>0.45</td>
<td>0.5</td>
<td>0.92</td>
<td>0.4565</td>
<td>2.0</td>
<td>0.5</td>
<td>1.0</td>
<td>1.5</td>
</tr>
</tbody>
</table>

### 3.4.3 Walls Impingement

The impact of particles, droplets or bubbles on rigid solid surfaces may produce a wide variety of consequences, according to the size, velocity and material of the impacting elements and the nature of the surface. For example, droplets may adhere, bounce or shatter and the liquid deposited on the surface may retain its droplet form or merge into a liquid film.

STAR-CD offers the following optional treatments of wall impact:

- Perfect rebound
• Adherence, either in the form of spherical droplets or as a liquid film. Droplet adhering to walls will exchange heat with them and will also continue to interact with the carrier fluid as far as heat and mass transfer is concerned.

• Instantaneous evaporation

*Bai’s spray impingement model*

This spray impingement model is formulated within the framework of the Lagrangian approach, on mass, momentum and energy conservation constraints. In order to reflect the stochastic nature of the impingement process, a random procedure is adopted to determine some of the droplet post-impingement quantities. This allows secondary droplets resulting from a primary droplet splash to have a distribution of sizes and velocities.

The current STAR-CD implementation assumes

• either wet or dry wall impingement

• elastic rebounding from walls whose temperature is greater than the boiling/critical temperature

There is a variety of impingement regimes, governed by a number of parameters such as

• incident droplet velocity relative to the wall

• incidence angle

• droplet size and properties

as well as

• wall temperature
• wall surface roughness
• liquid film thickness
• near-wall gas conditions

Some of the physical quantities involved are combined into dimensionless parameters, e.g.

• a variety of the droplet Weber number $We_d$ that uses droplet density and normal-to-the-wall components of relative velocities between the wall and the droplets
• the Laplace number, $L_a$, defined as

$$La = \frac{p_d \sigma_d D_d}{\mu_d^2}$$

(3.39)

Regime transition criteria

The model recognizes the following regimes:

• Stick – the impinging droplet adheres to the wall in nearly spherical form
• Spread – the droplet spreads out along the wall surface creating a wall film or merging with an existing film on a wetted wall
• Rebound – the impinging droplet bounces off the wall after the impact
• Splash – the impinging droplet breaks up into smaller droplets, some of which are reflected from the wall
For the sake of completeness, the transition criteria for both dry and wetted walls are given below:

1. Dry wall
   
   (a) Adhesion (combine with stick and spread regimes):
   \[ We_a \leq We_a \]

   Where \( We_a \) is:
   \[ We_a = \alpha L_a^{0.18} \]

   (b) Splash:
   \[ We_a > We_a \]

**Table 3-2: Dependence of Coefficient \( A \) on the wall surface roughness**

<table>
<thead>
<tr>
<th>( r_i [\mu m] )</th>
<th>0.05</th>
<th>0.14</th>
<th>0.84</th>
<th>3.1</th>
<th>12.0</th>
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<tbody>
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<td>4534</td>
<td>2634</td>
<td>2056</td>
<td>1322</td>
</tr>
</tbody>
</table>

3.5 Coupled Procedure

3.5.1 Introduction to Solution Algorithms and Flow Initialization

STAR-CD currently incorporates three different implicit algorithms, namely:

1. A variant of the well known SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) method,

2. The more recent and efficient PISO (Pressure Implicit with Splitting of Operators) method

3. The SIMPISO algorithm which, as the name implies combines elements of both the other methods.
3.5.2 The PISO algorithm

PISO is applicable to both transient and steady-state calculations and is particularly suitable for the former, for which it has been shown to be considerably more efficient than iterative methods.

1. It employ forms of predictor-corrector strategy, enabled by the use of operator splitting, to temporarily decouple the flow equations from each other so that they can be solved sequentially.

2. Continuity is enforced with the aid of an equation set for pressure, derived by combining the finite volume momentum and mass conservation equations.

3. The solution sequence involves a predictor stage, which produces a provisional velocity field derived from the momentum equation and a provisional pressure distribution. The provisional fields are then refined in the corrector stage by demanding simultaneous satisfaction, to some approximation, of both momentum and continuity balances.

4. Within the sequence, of the operator-split equation sets involve, at any stage, only one of the field variables, i.e. the vector set of unknowns is split into a sequence of scalar sets.

5. The algebraic equation sets are solved by iterative means.
**Working equations**

For the purpose of presentation, the FV momentum equations are extracted from the general transport equation in the form

\[ A_{ri}u_{i,p}^n = H(u_{i,m}^n) + B_{ri}u_{i,p}^n + s_i + D_r(p_{N+}^n - p_{N-}^n) \]  

(3.40)

Where

\[ H(u_{i,m}) = \sum A_{rn}u_{i,m} \]  

(3.41)

---

**Fig 3-1.** Arrangement of variables and notation for PISO implementation on Cartesian mesh

**Solution sequence**

Starting from initial value \( \phi^0 \) of the variable fields, PISO advances through a time increment \( \Delta t \) in the following sequence of steps.
1. **Predictor stage**  Equation [3.5.1] are assembled and solved in the following operator-split form for the provisional nodal velocity field $u_i^{(1)}$:

$$A_p u_i^n = H(u_{i,m}^n) + B_p^o u_{i,p}^o + s_i + D_p (p_N^{(o)} - p_{N-}^{(o)})$$  \hspace{1cm} (3.42)

Where $P^{(o)}$ corrector to the pressure field at the start of the time step. Following the solution of this equation, obtained by an iterative method, the provisional face velocities $u_j^{(1)}$ are calculated, with the $u_i^n$ and $P^n$ replaced by $u_j^{(1)}$ and $P^o$, respectively.

2. **First corrector stage.** The operative nodal momentum equation is now taken to be

$$A_p u_i^2 = H(u_{i,m}^1) + B_p^o u_{i,p}^o + s_i + D_p (p_N^{(1)} - p_{N-}^{(1)})$$  \hspace{1cm} (3.43)

And the face momentum equations are likewise approximated by replacing $u_j^{(o)}$ and $u_j^{(2)}$ and $P^{(i)}$, respectively. Correspondingly, the pressure equation in its approximated form reads.

$$A_p p_p^{(2)}(u_{i,m}) = \sum_m A_m p_m^{(1)} + s_i$$  \hspace{1cm} (3.44)

3. **Additional Corrector Stages.** Further corrector stages are calculated in the same manner as the first one, using the generalized equations.

$$A_p u_i^{(q+1)} = H(u_{i,m}^{(q)}) + B_p^o u_{i,p}^{(q)} + s_i + D_p (p_N^{(q)} - p_{N-}^{(q)})$$  \hspace{1cm} (3.45)

$$A_p p_p^{(q)}(u_{i,m}) = \sum_m A_m p_m^{(q)} + s_i$$  \hspace{1cm} (3.46)
Where \( q = 1, 2, \ldots \) is the corrector level. Note that \( A_p \) are held constant. The solutions from the successive stages represent increasingly better approximations to the solution of the original equations, i.e. \( u_j^{(q+1)} \) and \( P^{(q+1)} \) tend towards \( u_j^n \) and \( P^n \) with increasing \( q \).

After completion of the required number of correctors, judged according to practices described below, the solution produced is taken as the starting field for the next time step and the sequence is repeated from stage 1. If the calculation of scalar fields such as the turbulence parameters and temperature is required, it is performed in further steps executed after the final flow corrector. Alternatively, if the scalars are strongly coupled to the flow field through, for example, compressibility effects or combustion, they are embedded in the main predicator/corrector sequence.

3.6 Discretisation Practice

General Formation

The differential equations governing the conservation of mass, momentum, energy, etc. within the fluid are discretised by the finite volume method. Thus, they are integrated over the individual computational cells and then approximated in terms of the cell-centered nodal values of the discretised forms preserve the conservation properties of the parent differential equations.
For the purpose of the finite volume discretisation, the conservation equations:

\[
\frac{\partial}{\partial t}(\rho \phi) + \text{div}(\rho \vec{u}_r \phi - \Gamma_\phi \text{grad } \phi) = s_\phi
\]  

(3.47)

Where \( \vec{u}_r = \vec{u} - \vec{u}_c \) is the relative velocity between the fluid \( \bar{u} \) and the local coordinate velocity \( \bar{u}_c \). \( \phi \) stands for any of the dependent variables (i.e. \( u, e, k, m \) etc.) and \( \Gamma_\phi, s_\phi \) are the associated ‘diffusion’ and ‘source’ coefficients, which can be deduced from the parent equations.

An exact form of equation [3.6.1], valid for an arbitrary time-varying volume \( V \) bounded by a moving closed surface \( S \) can be written as:

\[
\frac{\partial}{\partial t} \int_V \rho \phi \, dv + \int_S \left( \rho \vec{u}_r \phi - \Gamma_\phi \text{grad } \phi \right) \cdot \vec{S} = \int_V s_\phi \, dV
\]  

(3.48)

where \( \vec{S} \) is the surface vector and \( \vec{u}_r \) is now the relative velocity between the fluid \( \bar{u} \) and the surface \( \bar{u}_c \). If \( V \) and \( S \) are, respectively, taken to be the volume \( V_p \) and discrete faces \( S_j, (j=1,N_j) \) of a computational cell equation [3.6.2] becomes

\[
\frac{\partial}{\partial t} \int_{V_p} \rho \phi \, dv + \sum_j \int_S \left( \rho \vec{u}_r \phi - \Gamma_\phi \text{grad } \phi \right) \cdot \vec{S} = \int_{V_p} s_\phi \, dV
\]  

(3.49)

**Temporal Discretisation**

The finite volume equation applies over an arbitrary time increment \( \delta t \) spanning the ‘old’ and ‘new’ time levels. Two options are available for temporal discretisation. The default option is a fully-
implicit scheme. An alternative second order Crank-Nicholson scheme may also be used.

**Fully implicit scheme**

Under this formulation, the fluxes prevailing over the time interval are calculated from the new time-level values of the variables.

In principle, the fully-implicit formulation allows any magnitude of time step to be used, but in practice other considerations impose limits i.e. for transient problems, \( \Delta t \) must be enough to limit the temporal approximation errors to acceptable levels.

### 3.7 Error Estimation

The error estimation gives an overview of the approximate magnitude and distribution of the discretisation error in the solution domain. The errors included in the estimate are caused by the mesh spacing, irregularity and non-orthogonality, the choice of the convection differencing scheme and the time-step size for transient calculations.

The residual error estimation method implemented in STAR-CD is based on the local imbalance between the face interpolation and volume integration, which produces a cell residual. The residual is normalized in an appropriate way to produce the estimate of the absolute magnitude of the error, with the same physical dimensions as the variable in question.
For the Navier-Stokes equations, the error is estimated for the velocity field, with the error in pressure distribution incorporated into the same the estimate. Although the residual error estimate provides the error in vector form, it is usually more intuitive to examine its magnitude.

In turbulence distribution and magnitude of the discretisation error can be obtained from the estimated error in the velocity and turbulence kinetic energy. If the near-wall regions is treated using wall functions, there may be some interference with the error estimation process, depending on the $y^+$ values and local mesh quality. If the residual error estimate for velocity produces an unrealistically high error near the wall, a special built-in procedure may be used to correct it. The error estimate in temperature, turbulence dissipation and other scalars can be included, depending on the nature of the flow.

### 3.8 Chemical Reaction and Engine Combustion Methodology

#### 3.8.1 Introduction

STAR-CD is applicable to chemically reacting flows because it provides for the solution of conservation equations for chemical species and energy. The package also allows for possible linkage with the flow field via density changes brought about by temperature and/or mass fraction variations.
The physical complications are mainly associated with issues of chemical kinetics, turbulence and their interactions. Chemical kinetics is concerned with the mechanisms and rates of reaction of chemical species at the molecular level.

Internal combustion engine problems require specialised modeling capabilities. While performing combustion calculations specific to internal combustion engines, the available facilities take into account the following features of engine process:

- Fluid dynamics, including turbulence
- Heat transfer
- Multi-component gaseous mixing
- Momentum, heat and mass exchange with droplets
- Auto-ignition and spark ignition
- Combustion
- Complex geometry
- Moving boundaries

A common assumption in flame-area models is that the flame is an infinitesimally thin surface which propagates in space while being affected by various physical processes, such as stretching, curvature and cusp formation. These processes are modeled through a transport equation for the flame is density or a related variable that describes the distribution of the flame surface.
3.8.2 ECFM Combustion Model[97]

The Extended Coherent Flame Model (ECFM) model is suitable for non-homogeneous premixed combustion and employs the conditional average technique. The model splits the combustion process into two parts:

- The premixed part, where the flame surface density equation is solved
- The post-flame part, where the Magnussen eddy break-up model is adopted

**Premixed Stage**

This stage deals with premixed combustion and the model’s equations are very similar to standard Coherent Flame Model.

**Flame area density**

The flame area (mass) density \( \sigma \) obeys a transport equation of the form:

\[
\frac{\partial \rho \sigma}{\partial t} + \nabla \cdot (\rho \sigma u) - \nabla \cdot \left( \frac{\mu_{eff}}{\sigma_{r,e}} \nabla \sigma \right) =
\]

\[
\left[ 2 \nabla \cdot u + \alpha T \frac{\varepsilon}{k} + \frac{2}{3} \frac{\rho_u}{\rho_b} \sum_i \frac{1-c}{c} - \beta U_i \frac{\varepsilon}{1-C} \right] \varepsilon \quad (3.50)
\]

Where \( c = 1 - \frac{Y_f}{Y_{r,f}} \) is the progress variable,

\( \bar{c} = 1 - \frac{(\rho Y_f)}{(\rho u Y_{r,f})} \) the Reynolds-averaged progress variable
The laminar flame speed, $U_l$ is computed

\[
U_l = S_{10} \left( \frac{T_u}{T_o} \right)^a \left( \frac{p}{p_o} \right)_b (1 - 2 \cdot 1X_{res})
\]

where $S_{10}$ is the adiabatic laminar flame speed at 300 K and 1 bar,

$a$ and $b$ empirical coefficients,

$p$ the absolute pressure,
\( p_0 \) and \( T_0 \) the reference absolute pressure (1 bar) and temperature (300 K), respectively, 
\( T_u \) the absolute temperature of the un-burnt gases, 
and \( X_{\text{res}} \) the mole fraction of the residual gases.

**Species transport equations**

The species mean mass fractions \( Y_i \) obey:

\[
\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i u) - \nabla \cdot \left( \frac{\mu_{\text{eff}}}{\sigma_{i,j}} \nabla Y_i \right) = \omega_i 
\]

where \( \omega_i \) and \( \sigma_{i,j} \) are the reaction rate and Schmidt number for species \( i \) respectively. In particular, for the fuel mass fraction:

\[
\frac{\partial \rho Y_f}{\partial t} + \nabla \cdot (\rho Y_f u) - \nabla \cdot \left( \frac{\mu_{\text{eff}}}{\sigma_{f,j}} \nabla Y_f \right) = \omega_f 
\]

where \( \omega_f = -\rho_a Y_{f,j} U_j \varepsilon \) (3.54)

The reaction rates for the other follow from the stoichiometry of the fuel-oxidation reaction.

**Source due to evaporation**

If fuel droplets are evaporating, the fuel mass fraction transport equation acquires the following additional source term:

\[
\omega_{f,\text{evap}} = (1 - c) \omega 
\]

where \( \omega \) is the fuel evaporation rate. Therefore the final form of \( Y_i \) is:
\[
\frac{\partial \rho Y_f}{\partial t} + \nabla \cdot (\rho Y_f u) - \nabla \cdot \left( \frac{\mu_{\text{eff}}}{\sigma_{t,i}} \nabla Y_f \right) = \omega_f + \omega_{f,\text{evap}}
\]  
(3.56)

The equation for \( \omega_{f,\text{evap}} \) indicates that only a fraction \((1-c)\) of the evaporated fuel is added to the fuel mass fraction \( Y_f \), the remaining part \((c)\) going into species 'fb' (fuel behind the flame).

The source term for the latter then reads:

\[
\omega_{f,\text{evap}} = c \omega
\]  
(3.57)

and the transport equation for its mass fraction \( Y_{fb} \) becomes:

\[
\frac{\partial \rho Y_{fb}}{\partial t} + \nabla \cdot (\rho Y_{fb} u) - \nabla \cdot \left( \frac{\mu_{\text{eff}}}{\sigma_{t}} \nabla Y_{fb} \right) = \omega_{fb} + \omega_{fb,\text{evap}}
\]  
(3.58)

Where \( \omega_{fb} \) is the reaction rate determined by the Magusses EBU model

**Tracer transport equations**

The tracers keep trace of species in the un-burnt gases. ECFM solves for two tracers, one for fuel \( Y_{T,f} \) and one for oxygen \( Y_{T,o_2} \). Their transport equations are:

\[
\frac{\partial \rho Y_{T,f}}{\partial t} + \nabla \cdot (\rho Y_{T,f} u) - \nabla \cdot \left( \frac{\mu_{\text{eff}}}{\sigma_{t}} \nabla Y_{T,f} \right) = \omega
\]  
(3.59)

\[
\frac{\partial \rho Y_{T,o_2}}{\partial t} + \nabla \cdot (\rho Y_{T,o_2} u) - \nabla \cdot \left( \frac{\mu_{\text{eff}}}{\sigma_{t}} \nabla Y_{T,o_2} \right) = \omega
\]  
(3.60)
**Thermal enthalpy transport equation**

In line with the reaction sources for species, the thermal enthalpy equation source term reads:

\[ \dot{\omega}_h = - \sum_i \omega_i (\Delta H)_i^0 \]  

(3.61)

Where \((\Delta H)_i^0\) the heat of formation for species \(i\).

The thermal enthalpy transport equation then reads:

\[ \frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h u) - \nabla \cdot \left( \frac{\mu_{\text{eff}}}{\sigma_{h,i}} \nabla h \right) = \frac{D_p}{\rho u} \frac{Dp}{Dt} + \rho \varepsilon + \omega_h + \omega_h + \omega_{h,\text{exp}} \]  

(3.62)

where \(\omega_{h,\text{exp}}\) is the source temp due to droplet evaporation.

**Enthalpy of un-burnt gases**

The transport equation for \(h_u\) reads:

\[ \frac{\partial \rho h_u}{\partial t} + \nabla \cdot (\rho h_u u) - \nabla \cdot \left( \frac{\mu_{\text{eff}}}{\sigma_{h,i}} \nabla h_u \right) = \frac{\rho}{\rho u} \frac{Dp}{Dt} + \rho \varepsilon + \omega_{h,\text{exp}} \]  

(3.63)

**Post-flame stage**

This stage deals with the diffusion part of the flame.

**Post-flame chemistry**

The post-flame section for chemical reactions that take place behind the flame, namely:

1. Post oxidation of species 'fb' (Magnussen EBU model)
2. Chemical equilibrium / dissociation
3. NOx (Z’eldovich extended mechanism)
All three sets of reactions above are calculated using the conditional burnt species $Y_b$ and burnt species enthalpy $h_b$.

**Mean properties update**

Once the burnt species $Y_{i,b}$ and burnt gas enthalpy $h_b$ have been computed in the post-flame stage, updated values for the mean mass fractions $Y_i$ and enthalpy $h$ are fractions $Y_{i,u}$ and the unburnt species enthalpy $h_u$:

\[
Y_i^{\text{new}} = (1-c)Y_{i,u} + cY_{i,b} \quad (3.64)
\]
\[
h^{\text{new}} = (1-c)h_u + ch_b \quad (3.65)
\]

**Ignition**

ECFM computes the delay between the spark discharge and the appearance of a flame kernel. After this delay, a flame kernel is determined, and the flame area density $\sigma$ and burnt gases are initialized and then distributed around the ignition location.

**3.8.3 ECFM-3Z:**

Compared to ECFM, ECFM-3Z offers an additional level of refinement involving the modeling of sub-grid turbulent mixing between air and fuel. This enables users to perform more accurate simulations of un-premixed (diffusion) combustion.
**Mixing model**

'3Z' stands for three zones of mixing, in which the local mixture is decomposed into

- the unmixed fuel \( Y_{fum} \),
- the unmixed air plus EGR gas (both are functions of the unmixed oxygen \( Y_{O_2,um} \)),
- the mixed gases.

The mixed gases are the product of mixing between the unmixed fuel and unmixed air + EGR. The decomposition is performed using a mixing model in which transport equations for the unmixed fuel and unmixed oxidizer are solved.

**General computational scheme**

The general process of computation is as follows:

- Calculation of the mixed quantities
- Combustion calculation (auto-ignition + premixed + post-flame)
  as in ECFM
- Reconstruction of the mean quantities

**Autoignition**

The autoignition model is based on the conditional unburnt mixed gases and it predicts the autoignition delay using an Arrhenious-type correlation.
An intermediate function $Y_{ig}$ is used to establish whether or not autoignition occurs. Once autoignition is reached, the mixed fuel is burned at a rate determined by a chemical characteristic time and a flame kernel is created. The autoignition model is also extended to encompass of cold flames.

**Premixed and post-flame stages**

Like auto-ignition, this part is also computed over the mixed gases as follows:

- The ECFM model is applied
- Equation (3.50) is used to compute the fuel consumption rate at the premixed stage.
- The post-flame stage is calculated afterwards

**Post-flame chemistry in ECFM-3Z**

The post-flame part in 3Z differs from its ECFM counterpart in the following ways:

- A kinetic reaction mechanism is introduced for CO and CO$_2$ mass fractions
- The ERC soot model is activated.

**EGR composition**

The EGR composition in ECFM-3Z is assured to consist of $N_2$, CO$_2$, H$_2$O, NO, CO, H$_2$ and soot. This differs from the standard ECFM
formulation, where the EGR mixture is assumed to include only $N_2$, $CO_2$ and $H_2O$.

**Regression model**

It is assumed that if the local burnt gas temperature falls below $1200K$, flame extinction occurs. In this situation, the regression model transfers burnt gas mass into unburnt gases (EGR) at the expense of the total fuel mass.

### 3.8.4 NOx Formation

Nitrogen oxides are important air pollutants, mainly produced by combustion devices. The $NOx$ concentration is low in most of these devices therefore; it has little influence on the flow field. Also, the time scale for $NOx$ reaction is larger than the time scales for the turbulent mixing process and the combustion of hydrocarbons that control the heat-releasing reactions. Hence, computations of $NOx$ can be decoupled from the main reacting flow field predictions.

Three different mechanisms have identified for the formation of nitric oxide during the combustion of hydrocarbons, namely:

1. Thermal $NOx$
   
   As its name suggests, it is strongly temperature dependent. It is produced by the reaction of atmospheric nitrogen with oxygen at elevated temperatures.

2. Prompt $NOx$
The exact details of prompt NOx formation are still uncertain but are generally believed to involve the reactions between hydrocarbon radicals and atmospheric nitrogen. In certain combustion environments (such as low-temperature, fuel-rich condition and short residence time), prompt NOx can be produced in significant quantities.

3. Fuel NOx

This is produced by the reaction of the nitrogenous components present in liquid or solid fossil fuel with oxygen. The fuel nitrogen is a particularly important source of nitrogen oxide emissions for residual fuel oil and coal, which typically contain 0.3 – 2.0% nitrogen by weight.

**Thermal NOx**

Thermal NOx is formed by high temperature oxidation of atmospheric nitrogen. For thermal nitric oxide, the principal reactions are generally recognized to be those proposed by the following three extended Zeldovich mechanisms:

\[
N_2 + O \xrightarrow{k_1} NO + N \quad (3.66)
\]

\[
N + O_2 \xrightarrow{k_2} NO + O \quad (3.67)
\]

\[
N + OH \xrightarrow{k_3} NO + H \quad (3.68)
\]

The rate constants for these reactions have been measured in numerous experimental studies, and the data obtained from these
studies. The expressions for rate coefficients for reactions are given below:

\[ K_1 = 1.8 \times 10^{11} \exp\left(-\frac{38370}{T}\right) \quad m^3 (kg \ mol^{-1}) \ s^{-1} \quad (3.69) \]

\[ K_{-1} = 3.8 \times 10^{11} \exp\left(-\frac{425}{T}\right) \quad m^3 (kg \ mol^{-1}) \ s^{-1} \quad (3.70) \]

\[ K_2 = 1.8 \times 10^{7} T \exp\left(-\frac{4680}{T}\right) \quad m^3 (kg \ mol^{-1}) \ s^{-1} \quad (3.71) \]

\[ K_{-2} = 1.8 \times 10^{6} T \exp\left(-\frac{20820}{T}\right) \quad m^3 (kg \ mol^{-1}) \ s^{-1} \quad (3.72) \]

\[ K_3 = 7.1 \times 10^{10} \exp\left(-\frac{450}{T}\right) \quad m^3 (kg \ mol^{-1}) \ s^{-1} \quad (3.73) \]

\[ K_{-3} = 1.7 \times 10^{11} \exp\left(-\frac{24560}{T}\right) \quad m^3 (kg \ mol^{-1}) \ s^{-1} \quad (3.74) \]

where \( K_1, K_2 \) and \( K_3 \) are the forward and \( K_{-1}, K_{-2} \) and \( K_{-3} \) are the backward rate constants for reactions, respectively.

The rate of formation of NOx is significant only at high temperature since the thermal fixation of nitrogen requires the breaking of a strong \( N_2 \) bond. This effect is represented by the high activation energy of reaction, which makes this reaction the rate-limiting step of the Zeldovich mechanism. The activation energy for oxidation of N is small hence a quasi-steady can be established. Based on this assumption, the instantaneous of NOx is:
\[
\hat{R} = \frac{\rho^2}{1 + K_1 \frac{Y_{NO}}{M_{NO}} \left( K_2 \frac{Y_{O_2}}{M_{O_2}} + K_3 \frac{Y_{OH}}{M_{OH}} \right)}
\]

\[
\begin{bmatrix}
2K_1 \frac{Y_O}{M_O} \frac{Y_{NO}}{M_{NO}} - \frac{2K_1 Y_{NO}}{M_{NO}} \left( K_2 \frac{Y_{O_2}}{M_{O_2}} + K_3 \frac{Y_{OH}}{M_{OH}} \right) \\
k_{NO}^2
\end{bmatrix}
\]

\(\text{kg mol m}^{-3} \text{s}^{-1}\) \hspace{1cm} (3.75)

If the mass fraction of radicals \(O\), \(OH\) and \(H\) are calculated by the combustion model, they are used in the \(NOx\) model. Otherwise, certain assumptions have to be made to obtain their values. For example, according to Westenberg, the equilibrium \(O\) atom mass fraction can be obtained from:

\[
[O] = K_o [O_2]^{1/2} \text{ kg mol m}^{-3} \hspace{1cm} (3.76)
\]

and

\[
Y_O = [O]^2 \frac{M_O}{\rho} \hspace{1cm} (3.77)
\]

Where

\[
K_p = \frac{3.97 \times 10^5}{T^{1/2}} \exp \left( -\frac{31090}{T} \right) \text{ (kg mol)}^{1/2} \text{ m}^{3/2}\] \hspace{1cm} (3.78)

In the mass fraction of \(O\) atoms is obtained from equation [3.8.27] and those of \(OH\) and \(H\) are initially set to zero.
Prompt NOx

Prompt NOx is formed from the reaction of hydrocarbon fragments and molecular nitrogen. It has weak temperature dependence and a lifetime of only several microseconds. The contribution to NOx emission from this mechanism can be significant in systems that produce very fuel-rich flame (e.g. staged combustion system). In utility furnaces, prompt NOx contribution to total NOx is very small when compared with fuel NOx. However, the significance of prompt NOx is expected to increase as NOx emission levels are reduced continuously by new combustion technologies.

The production rate of prompt NOx is given by De Soete as,

\[ R_{NO,p_t} = k_{pt}M_{NO} \text{ kg m}^{-3}\text{s}^{-1} \] (3.79)

Where \( k_{pt} \) is a rate constant and is defined as:

\[ k_{pt} = k_r [O_2] [N_2][Fuel] \exp \left( \frac{-E_a}{RT} \right) \text{ kg mol m}^{-3}\text{s}^{-1} \] (3.80)

\([O_2], [N_2]\) and \([Fuel]\) are species concentrations in kg mol/m\(^3\). For \(C_2H_4\) air flames, the activation energy \(E_a\) is equal to 303.5X10\(^6\) J/kg mol. The universal gas constant \(R\) and temperature \(T\) and are in SI units. The oxygen reaction order, \(b\), depends on experimental conditions. According to De Soete, \(b\) varies with the oxygen mole fraction \(X_{O_2}\) as follows,

\[
\begin{align*}
  b &= 1.0 \quad X_{O_2} < 0.0041 \\
  b &= -3.95 - 0.9\ln X_{O_2} \quad 0.0041 \leq X_{O_2} \leq 0.0111 \\
  b &= -3.95 - \ln X_{O_2} \quad 0.0111 \leq X_{O_2} \leq 0.03
\end{align*}
\]
\[ b = 0.0 \quad \text{and} \quad X_{O_2} \geq 0.03 \]

### 3.8.5 Soot Modeling

The formation and emission of carbonaceous particles is a process that is often observed during the combustion of hydrocarbons. These particulates, called soot, are identified in flames and fires as yellow luminescence.

It is require a detailed knowledge of the different mechanisms leading to soot formation. It is widely accepted that the formation of soot is a complex process which consist of

- fuel pyrolysis and oxidation reactions
- formation of polycyclic and aromatic hydrocarbons
- the inception of first particles
- the growth of soot particles due to reaction with gas phase species
- the coagulation of particles
- the oxidation of soot particles and intermediates

**Mathematical model**

In this model, an additional transport equation for the soot mass fraction is solved for. The modelling of the soot/flow-field interaction is based on a flamelet approach. Source terms for the soot volume fraction are taken from a flamelet library using a presumed probability density function and integrating over mixture fraction...
space. In order to save computer storage and CPU time, the flamelet library of source is constructed using a multi-parameter fitting procedure resulting in simple algebraic equations and a proper set of parameters.

The transport equation for soot mass fraction is given by

$$\frac{\partial}{\partial t} (\rho Y_s) + \frac{\partial}{\partial x_j} (\rho u_j Y_s) = \frac{\partial}{\partial x_j} \left( \frac{\mu_s}{\text{Pr}_{s,s}} \frac{\partial Y_s}{\partial x_j} \right) + \rho_i \omega_s \tag{3.81}$$

Where $Y_s$ is the soot mass fraction. The Prandtl number for soot is assumed to be 1.4 and the soot density $\rho_i = 1860 \text{ ks/m}^3$. 