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Introduction

In recent years, due to the growth of powerful computing resources, the development of robust computational models and efficient algorithms has led to develop detailed models able to describe the behaviour of single component and of complex plants.
Two different approaches can be followed:

- Component behaviour is described by Input-Output relationships that can be represented and implemented by global equations;

- Component behaviour is described by models simulating the physical behaviour of machines and apparatuses. Different goals can be taken into consideration:

  - preliminary thermodynamic evaluations of cycle processes by taking global parameters into account;

  - determination of sizes that represent the design of machines and apparatuses at the nominal conditions. Such models are oriented to machines and apparatuses performance calculations taking also governing equation source terms (work exchange, heat transfer, entropy production, species etc.) into consideration. Empirical relations based on manufacture and user data, technical literature background and so on, can be taken into account;

  - component and plant off design and part load behaviour analyses under steady-state and transient conditions can be calculated.

Nowadays, plant behaviour can be described by elementary modules representing single components or macro modules describing the behaviour of complex plant sections. To represent the plant such modules are matched together. Various platforms allow an easy build-up of the plant but the component models quite often can be adapted to new machines and apparatuses with some difficulties.

In the following paragraphs, a survey of models of components available at the partner sites is presented.

Component Models available at ROMA TRE University

RO3, in connection with past EU Projects, has developed models that have shown to be valid and flexible.

Such RO3 models are easily adaptable to new components and can allow the introduction of modifications for machines and apparatuses.

Background

Each thermo-mechanical system usually is made of many components each of which is devoted to one process transfer of heat, of work, of combustion etc. Closed loop plants or equivalent ones (like IGCC plants, steam cycles, gas turbines, combined cycles, etc.) can be plotted as in figure 1, where blocks 1, 2 ... represent components or group of them. In such a figure connections between components, input and output streams are schematically represented (E_{In}^U being the vector of the useful inlet quantity fluxes, E_O^U being the vector of fluxes of useful quantities, while E_O^R being the vector of fluxes of rejected quantities).

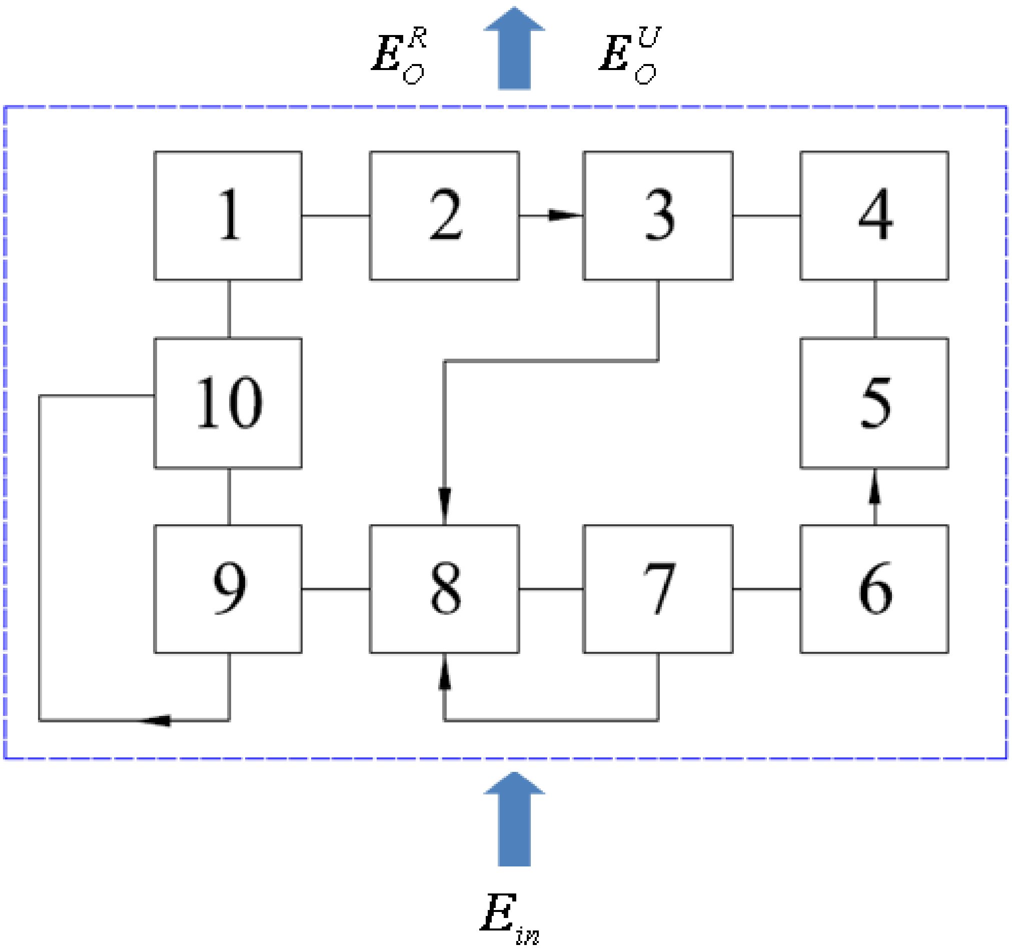


Figure 1: Generic plant diagram

Behaviour of a generic plant can be described by an equation set:

$$\boldsymbol{F}(z) = 0 \tag{1}$$

and by an inequality set:

$$\boldsymbol{D}(z) \geq 0 \tag{2}$$

being $\boldsymbol{z}$ the overall variable set:

$$\boldsymbol{z} = \boldsymbol{y} \cup \boldsymbol{b} \cup \boldsymbol{u} \cup \boldsymbol{g} \tag{3}$$

being $\boldsymbol{y}$ the variable set:

$$\boldsymbol{y} = \boldsymbol{\xi} \cup \boldsymbol{x} \tag{4}$$

made by independent variables $\boldsymbol{\xi}$ (*DOFs)* and by unknown variables ***x****.*
b is the boundary conditions set (ambient, etc.) and ***u*** is the status of the system set.

In general, equations ***F*** are highly non linear and express conservation of mass, momentum, energy and entropy, and other phenomena such as work and heat transfer, combustion, pressure loss, etc. ***F*** includes also fluid properties, auxiliary equations, machine and equipment specifications. Equations can also be expressed in terms of graphs or tables. ***D*** represents a set of physical, thermal, chemical and geometrical conditions, as well as other constrains which determine the domain where the problem (2.1) solution exists.
The values associate to the vector $\boldsymbol{\xi}$ components usually is establish ξ_k according to suitable criteria one of which can be the search of an appropriate objective function optimum value. X is the solution of (1) and (2). Of course quantities can be exchanged between $\boldsymbol{X}$ and $\boldsymbol{\xi}$.
The status of the system set **u** is made by r_f and a_f which are the vectors of realty functions and actuality ones respectively.

$$\boldsymbol{u} = \boldsymbol{r}_f \cup \boldsymbol{a}_f \tag{5}$$

Reality functions r_{fs} are introduced to accommodate the model to reproduce the existing component behaviour in a reference situation (*New & Clean*). Since during operations the component features behaviour change continuously due to various phenomena leading to performance modification, the model of each component has to be tailored to the new situation. Therefore the models of the major components include suitable *actuality functions* a_{fs} that can represent the actual status of the component. a_f takes into account the deviation of the actual component performance from a condition assumed as the reference.

Thermo-mechanical systems are described adopting a modular approach. This means that each component, or group of components, is described by a module whose structure may be defined by one or more subroutines. Each subroutine contains the model of the corresponding elementary unit (i.e. a compressor blade row, heat exchanger zone and so on). Complex components are built up linking various subroutines as macro-components (i.e. waste heat recovery system is built up calling the subroutines for all the requested sections).

Component and lumped features and performance

RO3 modelling approach is based on a Finite Volume (FV) lumped feature and performance discretisation of components. The approach is addressed to model any kind of machines and apparatuses made of elementary components such as: compressor rows, expander rows, combustion chambers, heat exchangers, pumps, etc. Taking the compressor as an example, a generic row by row scheme as reported in figure 2 is taken into consideration.

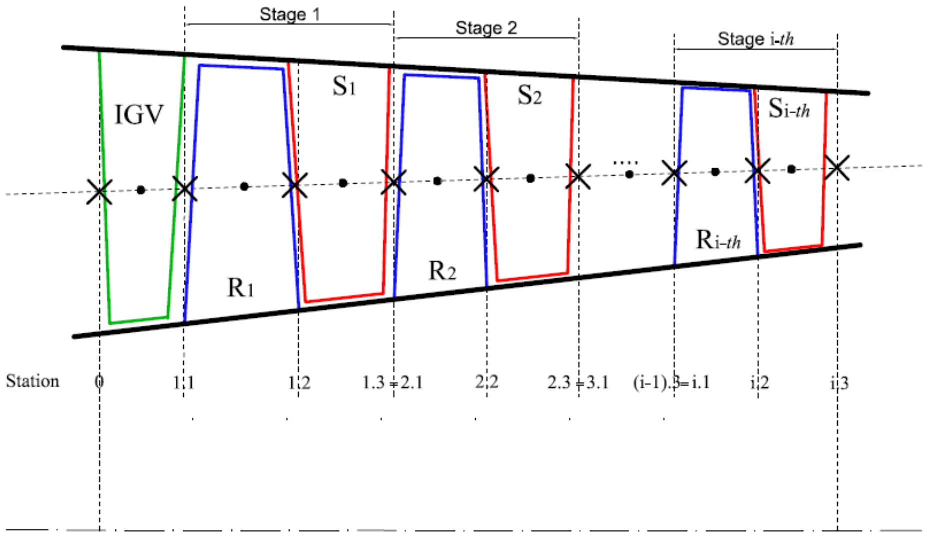


Figure 2: Generic compressor row by row scheme

The compressor is divided into each representing a stator or rotor cascade. Each row is included in finite volumes FV's delimited by a boundary, as figure 2.3 shows.

The inlet station and the central node are described by the same number J .

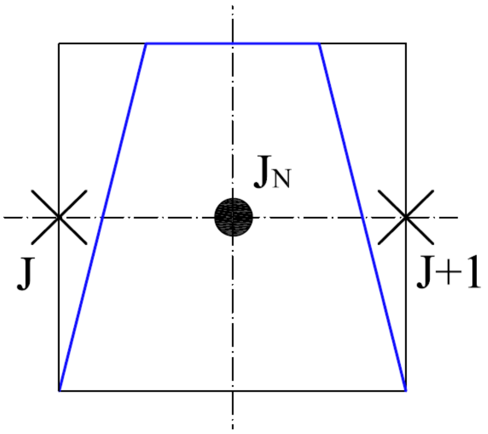


Figure 3: Finite Volume Row – Stations and central Node

Real three dimensional time dependent measured flow features are taken into account by lumping on the *FV* boundary models J and $J+1$ the distributions of quantities of interest such as pressure, velocity, temperature, etc., by means of an averaging procedure on surface and time. Moreover the lumping procedure is adapted for the quantities that are involved in the component performance calculation according to the implemented modules. The lumped features are reduced to the *FV* central nodes J_N. A scheme of a compressor model is given in figure 2 with the Blade Row Finite Volume scheme given in figure 3. Similar approaches are adopted for other devices. e.g. a heat transfer device such as a *shell & tube* heat exchanger can be modelled according to the *FV* elementary device given in figure 4a. For a condenser the *FV* approach leads to a multi-zone heat transfer device depicted in figure 4b.

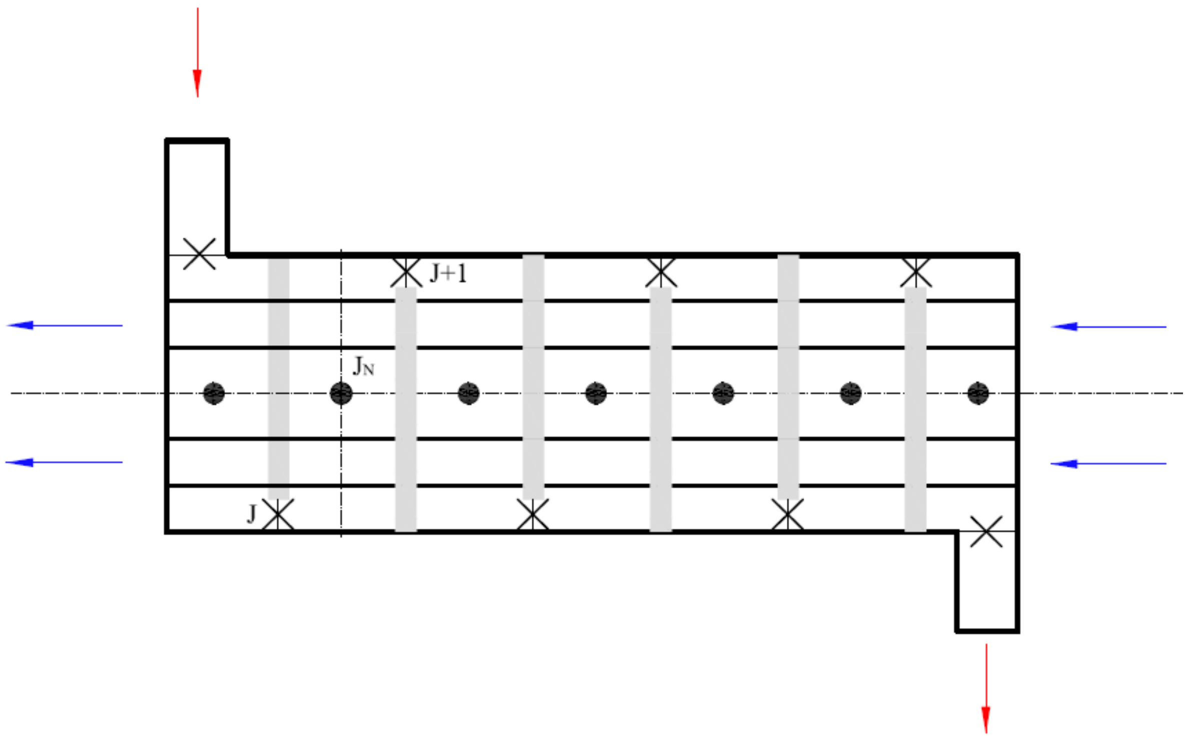


Figure 4a: Tube Bundle – Stations and central Node

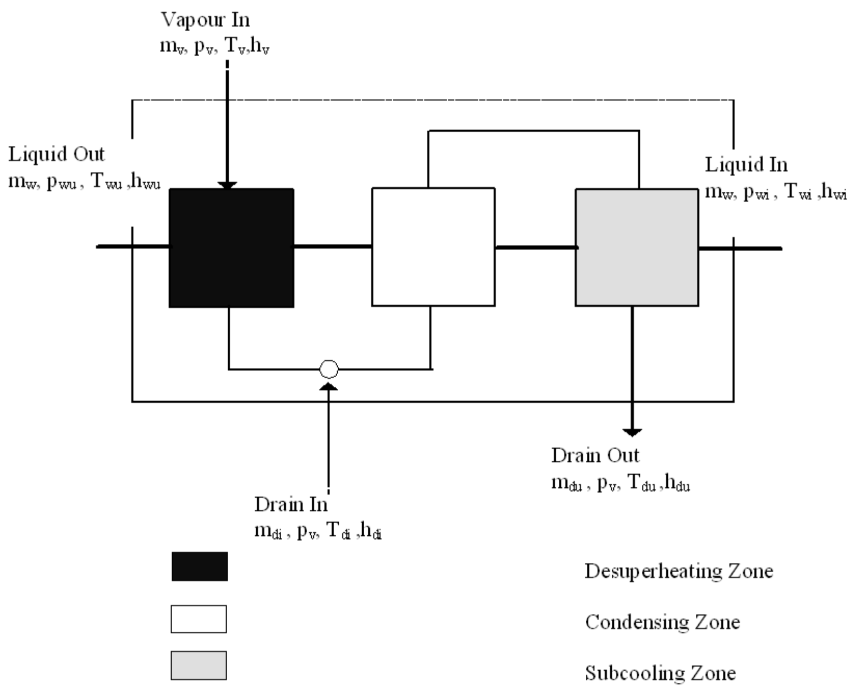


Figure 4b: Condenser – Multi-zone heat transfer device

Methodological Approach

Equations and inequalities describing machines and plant behaviour are addressed to solve different kind of problems. RO3 methodology is based on different steps:

- Cycle Calculation: this procedure is related to preliminary cycle calculation whet the cycle potentials are going to be investigated with only few constraints concerning thermodynamic quantities. Data are usually related to the state of the art machinery and equipment's (i.e. efficiency, heat transfer effectiveness and so on). If related to such above quantities cost specifications are available an optimization procedure can take place. Thermodynamic optimisation is always possible. Indeed overall plant efficiency and specific of work or a combination of these quantities may be chosen as objective function. Results of this calculation are thermodynamic quantities at some plant stations, mass flows, value of powers crossing component boundaries and overall performances.

- Sizing: this phase is preliminary to the next component off design component and plant part load analyses. It consists in the calculation of size of machines and equipment's and alternative global parameters to describe off-design behaviour of components. Input data are from the previous cycle calculations or may come from data base DB related to the commercially available machines and equipment's whose design features are close to that of required cycle calculation. In this phase specifications concerning costs of machines and equipments are used for optimized design. Results of this inverse calculation phase may be devoted to equipment and machine preliminary designs, but at present, they are mainly addressed to the next plant off-design investigation.

- Off-Design Analysis: this direct phase investigation requires the knowledge of geometric data, architecture and some global parameters related to the plant components. Maps of the machine and equipment are obtained and how they match in the plant is studied. Changes in the independent quantities (DOF's) may be investigated according to control policies the related rules may be implemented as specifications. In this casa the component state quantities (u) may be used to optimize operations according with load requirements (electric and thermal power) which are implemented as time dependent constraints.

Solution strategy

Once the parameters **u** and the degree of freedom **y** have been given, the search of the unknowns **z** may be performed by minimization of the ***plant unbalance function***.

$$\Delta(z) = F(z)^T F(z) \tag{6}$$

When the solution of $F(z)$ is achieved (i.e. $z = \bar{z}$), $\Delta(z)$ is zero.

The necessary condition $\Delta(z)$ minimum is achieved, the following **n** equations have to be satisfied.

$$\sum_{j=1}^{n} f_j \frac{\partial f_j}{\partial z_i} = 0 \quad \forall\, i \in [1, n] \tag{7}$$

Of course, this occurs when:

$$f_j(z^*) = 0 \;\forall\, j \in [1, n] \tag{8}$$

In this case, the Hessian matrix of $\Delta(z)$ is definite not negative for $z^* = \bar{z}$

$$\frac{\partial f_j(z^*)}{\partial z_i} = 0 \;\forall\, j \in [1, n] \tag{9}$$

In this case z^* is a stationary point for function $f_j(z)$, therefore, it may not be the searched solution point.

The above suggests the idea that stating the following minimization problem

$$\textbf{minimize}\ \{\Delta(z) |\ F(u, z, y) = 0; D(u, z, y) \geq 0; u = u^{\dagger *} \quad y = y^{\dagger *}\} \tag{10}$$

The solution of $F(u, z, y) = 0$ with $D(u, z, y) > 0$ is assumed because constraints of the minimization problem are both equations $F(z)$ and inequalities $D(z)$.

At any k-th step, $\Delta(z)$ represents the plant unbalance that vanishes when the solution is achieved.

Objective function definition

In order to solve problems of sizing, optimization, matching an appropriate algorithm (ECRQP) for the search of the minimum of an objective function has been adopted. In relation to the issues addressed, the objective function takes on different expressions. Indeed a set of objective functions $fob \in R^n$ may be established. The global objective function Fob is

$$Fob = \sum_{j=1}^{N} w_j \cdot fob_j \tag{11}$$

The first element, for $j=1$, represent the unbalance Δ ($\Delta = 1 \cdot fob_1$), the other elements may express a special objectives (like initial cost, operating cost, volume, weight, etc.) and weight vector elements w^T can take the value zero or one. Of course w_1 always must be 1.

Adopting the suitable formulation of the objective function Fob and the vector of unknown quantities $\boldsymbol{z}$ the following problem may be solved:

Search $z : \min \left\{ Fob \middle| F(\xi, x, b, u, g, r_f, a_f) = 0; D(\xi, x, b, u, g, r_f, a_f) \geq 0 \right\}$ (12)

Matching constraints and therefore plant unbalance are still taking into consideration.

Solution Methods

Various optimisation techniques based on Equality Constraint Recursive Quadratic Programming (ECRQP), Genetic Algorithms (GA) and Simulated Annealing (SA) as well as hybrid GA-ECRQP and SA-ECRQP have been applied and compared (Cerri, 1996; Cerri et al., 2005; Boccaletti et al., 2000). The choice of the most suitable one depends on the peculiar problem to be solved.

Simultaneous

Simultaneous means that all the unknown variables are foreseen (i.e. each assume a proper value) at the beginning of any step (iteration). Since all the unknown quantities are assumed in the iteration (see fig. 5) the contributions of all the component to the objective function (components unbalance, costs, etc.) and to the constraint structure may be calculated. Therefore the plant performance (when it is under an unbalanced condition), costs, emissions of pollutants and the objective function are evaluated. All components are described by equations which express: conservation of energy, mass, momentum and entropy (second thermodynamic law); other phenomena on physical or empirical basis such as work and heat transfer, pressure loss, etc.; fluid properties and auxiliary equations.
Components are described by algebraic relationships and by differential equations which are reduced to algebraic ones by adopting a finite difference procedure. Performance of a plant component is related to its load level. This relationship is influenced by its history (ageing, deterioration, fouling, maintenance and so on).
Problem (4) could be solved adopting an optimisation technique developed by Cerri (1991, 2010) based on ECRQP that provides to introduce two merit functions:

- the penalty function:

$$P(z,r) = Fob(z) + \frac{1}{r} \cdot v^T v \tag{13}$$

r being the penalty parameter and v being the vector of active constraints.

- the Lagrange function:

$$L(z,\lambda) = Fob(z) + \lambda^T v \tag{14}$$

λ being the set of Lagrange multipliers related to the constraints.

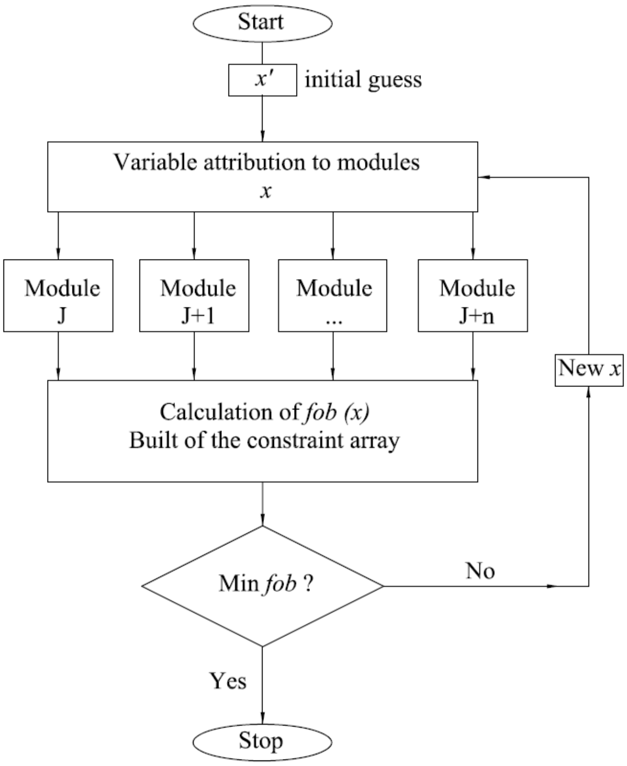


Figure 5: modular structure calculation method – ECRQP

The parameter r must be positive and when it tends to zero the minimum of $P(z,r)$ tends to the minimum of *Fob*. The minimum of $L(z,\lambda)$ also coincides with the minimum of *Fob*.

The solution is found starting from an initial tentative solution x_0. At the generic k^{th} iteration the step d_k (which moves the tentative solution from z_k to $z_{k+1} = z_k + d_k$) is searched by solving a quadratic-programming problem. The objective function is a quadratic approximation of Fob:

$$F_q = f_k d_k + \frac{1}{2} d_k^T d_k H_k \qquad (15)$$

f_k being the gradient of the Fob and H_k its Hessian matrix, both evaluated at point z_k. Second order Taylor's series expansion around z_k lead to approximate expression of the penalty function gradient:

$$\nabla P(z_k, r_k) = f_k + H_k d_k + \frac{2}{r_k}(A_k^T v_k + A_k A_k^T d_k) \qquad (16)$$

and the Lagrange function gradient:

$$\nabla L(z_k, \lambda_k) = f_k + H_k d_k + A_k^T \lambda_k \qquad (17)$$

A_k being the Jacobian matrix of active constraints calculated for $z = z_k$.

The search of d_k is performed by imposing the condition of minimum $P\,(\nabla P(z_k, r_k) = 0)$ and using further conditions resulting by equating the right terms of Eqs. (2.16) and (2.17). Therefore the steps towards the minimum of $Fob\,(z)$ are performed along the locus of penalty function minima, as shown in figure 2.6.

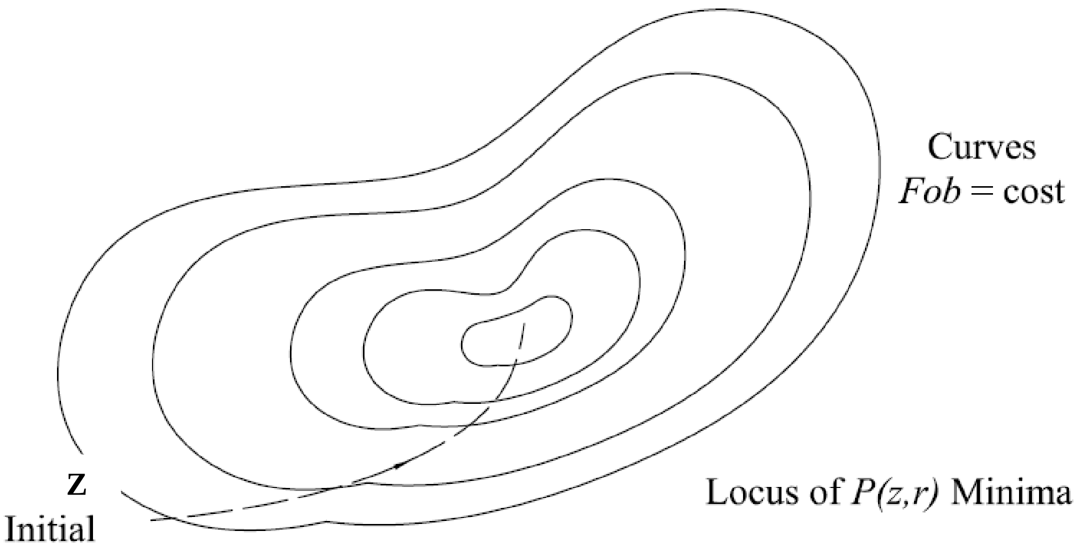


Figure 6: Solution Path along the Locus of P(z,r) Minima

Sequential

The most widely adopted method is the sequential one, by this method the plant is divided into modules corresponding to the plant components. For each module subsets of equations and inequalities are established. Each module is analysed sequentially, module outputs are solved from input quantities. Two major aspects related to the computing time have to be pointed out. The first is connected with the non linearity of the module equations which require internal iterations to get outputs. The second is related to closed loops and recycling streams (i.e. when the module under analysis needs other not yet analysed module outputs means that those variables have to be given as tentative ones, therefore external iteration levels in order to have balanced solutions of subsystem process groups). From given data, usually the solution starts from one module and continues following one fluid streams.

Due to the component equations being non-linear and really numerous for complex plants, various level (nested) iterative loops are needed. This method requires a big computation effort and a long CPU time.

Hybrid

The hybrid process consists in the division of the variables into different sets: one is the Dependent Variables *DV* that are the unknowns of the independent equation set; the second variable set consists in the Independent Variables *IV* that have to be given *a priori*_and do not change during the calculations. The *IV* set is made of the degree of freedom *DOF's* and of the Boundary Variables *BV or* $\boldsymbol{\beta}$ such as ambient conditions and similar ones. The hybrid approach consists in dividing the calculation environment into two zone. In the first zone, the *IV* set is established and the final outputs are saved. The second zone consists in the calculation of the *DV* set using the Non Linear Equation Solution *NLES* that can be performed by a simultaneous or sequential approach. This hybrid methodology is suitable also for the solution of optimization problems. In this case, the *DOF* set is divided in two sets. One is $\boldsymbol{\xi}$ that consists in the *DOF*'s to be optimized and the remaining *IV*'s consists in the $\boldsymbol{\beta}$ set whose components β_k remain constant during the calculations.

Accordingly, there are three zones:

- the first zone inputs inside the calculation process a suitable $\boldsymbol{\xi}^{\boldsymbol{j}}$ and calculates the related objective function;
- the second zone inputs into the calculation procedure the $\boldsymbol{\beta}$ set;
- the third zone provides the calculation of the unknowns by a simultaneous or a sequential procedure

Maps of the plant can be calculated by suitably changing the point inside the β domain.
The above procedure is implemented by RO3 Research Unit by adopting Genetic Algorithm *GA*, Simulated Annealing *SA* and *ECRQP.* The *GA-ECRQP* hybrid algorithm is schematically represented in figure 7.

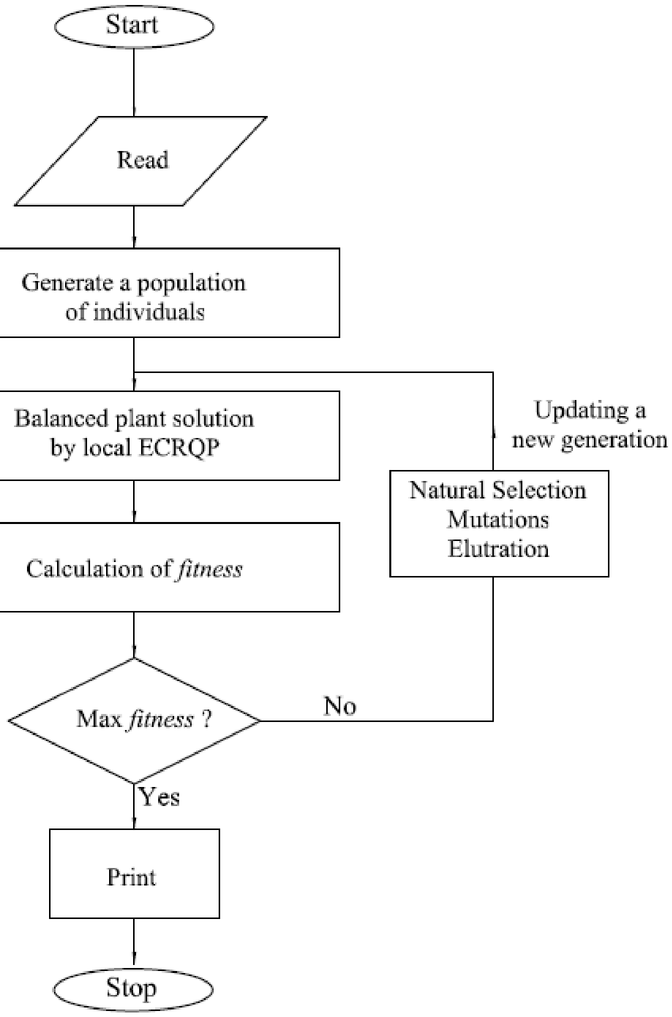


Figure7: Hybrid methodology – Genetic Algorithm/ECRQP

Modular approach

A thermo-mechanical system may be described by modules each corresponding to a component or sub-component of a plant. Each module exchanges with the other sections some information (Figure 8) which are input and output quantities and attributes like the component architecture and geometry in a direct problem.

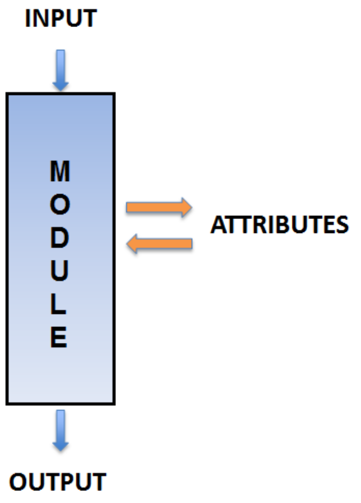


Figure 8: Module description

The set of equations **F** and inequalities D of each module can be split in subsets of equations

$$\Phi_j(d^{MJ}, x^{MJ}) = 0 \tag{18}$$

and of inequalities

$$\delta_j\,(d^{MJ}, x^{MJ}) = 0 \tag{19}$$

Of course, the above subsets must satisfy the following conditions

$$\boldsymbol{F} = \Phi_1 \cup \Phi_2 \cup \Phi_j \cup \Phi_z \tag{20}$$

and

$$\boldsymbol{D} = \delta_1 \cup \delta_2 \cup \delta_j \cup \delta_z \tag{21}$$

Each pair Φ_j, δ_j represents a module that can be a real component or a fictitious one; z being the number of modules.

A module is schematically represented in Figure 9 variables x^{MJ} are input; output quantities are:

- values assumed by equalities Φ_j, and inequalities δ_j;
- partial plant unbalance (component unbalance) Δ_j;
- other partial objective functions which represent component contributions fob_j
- other quantities of interest.

Due to the peculiarities of the simultaneous solution method, implementation of component specifications, which generally are function of both component inlet and outlet quantities, is really simple in these modules.

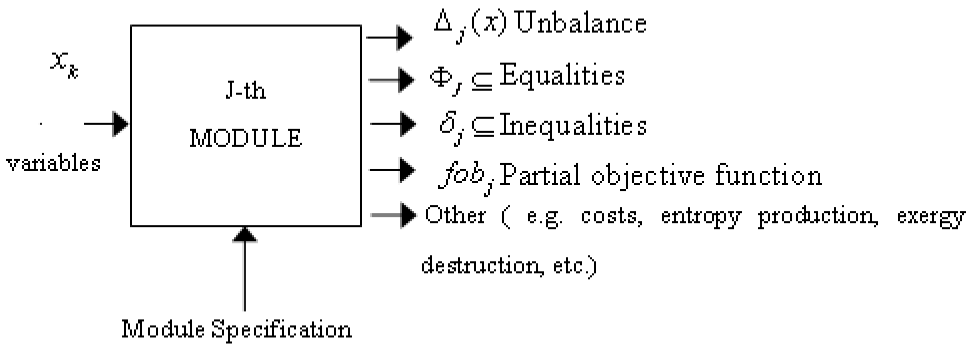


Fig. 9: Schematic Module Specification

List of RO3 models
The list below shows the models available at RO3 and developed on its own.

- Fluid Properties
- Weather Hood
- Air Filter
- Evaporative Cooler
- Coil
- Compressor
- Combustion Chamber
- Expander
- Diffuser
- Ducts connecting GT components
- Steam generators
- Heat Recovery Steam Generator (HRSG)
- Superheater
- Boiler
- Economizer/Preheater
- Postfire
- Steam Turbine
- Steam/water surface heat exchangers
- Deaerator
- Storage Vessel
- Pump
- Attemperator
- Gassifier
- Process compressors, fans and pumps
- Fluidized beds
- Heat Exchangers
- Junctions
- Valves
- Splitters
- Mixers
- Electric power generator
- High temperature solar receivers

Description of the models (examples)

Fluid Properties
Fluid properties routines have been derived by those already existing at RO3. Improvements concerning easy and fast utilization and more accurate description (such as the influence of ambient pressure on humid air properties). The amount of water vapour existing in the air varies with different conditions. Gas mixtures (e.g. O_2, N_2, CO_2, H_2O) with emphasis to air and combustion gases have been taken into consideration.
In this context revision of fluid properties have been done to identify the state of the flow (which may be in a mono-phase or two-phase flow) and routines have been improved to calculate thermodynamic properties at different conditions. Special modifications have been carried out by RO3 to allow the functions calculated from the two sites, wet and superheated, to have the same value on the dry saturated steam line.

Properties of two phase flow system
As discussed above, the air contains water, which could be in the form of vapour phase and liquid phase. Thermodynamically it is a difficult task to obtain the properties of the mixture undergoing a phase change. However assuming thermodynamic equilibrium for the system the properties of the mixture can be obtained, based on the following concepts:

Specific heat at constant pressure for two phase flow

The specific heat of a two phase flow mixture at equilibrium is defined as the rate of change of enthalpy with respect to temperature at constant pressure, i.e.

$$c_p = [\frac{dH}{dT}]_p \tag{22}$$

Since the enthalpy of the mixture at equilibrium is the sum of the enthalpies of the chemical species in the gas phase and enthalpies of the liquid phase, i.e.

$$H = m_g h_g + m_l h_l \tag{23}$$

where (g) and (l) denote the gas phase and liquid phase in the system.

$h_g = f$ (T_i, p_i, mass fraction of chemical species in the gas phase) (24)

$h_l = f$ (T_i) (25)

Thus, the specific heat of the system is given by:

$$c_{p_{sys}} = \frac{d(m_g h_g)}{dT} + \frac{d(m_l h_l)}{dT} \tag{26}$$

Being

$$m_g + m_l = \text{constant}$$

which implies that

$$\frac{dm_g}{dT} = -\frac{dm_l}{dT}$$

thus, eq. 26 can be written as

$$c_{p_{sys}} = m_g \frac{dh_g}{dT} + m_l \frac{dh_l}{dT} + (h_l - h_g)\frac{dm_l}{dT} \tag{27}$$

Note that the first term in the right hand side of eq. 27 indicates the specific heat of the chemical species in the gas phase, the second term indicates the specific heat of liquid phase, and the last term indicates the rate of change of liquid to vapour phase at constant pressure.
Hence, the specific heat of the system can be expressed as:

$$c_{p_{sys}} = \frac{H_2 - H_1}{T_2 - T_1} \tag{28}$$

where (H_2) denotes enthalpy at temperature (T_2) and (H_1) is the enthalpy at (T_1).

<u>Specific heat at constant volume for two phase flow</u>
The specific heat of a two phase flow mixture at equilibrium is defined as the rate of change of internal energy with respect to temperature at constant volume, i.e.

$$c_v = [\frac{dU}{dT}]_v \tag{29}$$

Since the internal energy of the mixture at equilibrium is the sum of the internal energy of the chemical species in the gas phase and internal energy of the liquid phase water, i.e.

$$U = m_g u_g + m_l u_l \tag{30}$$

Being:

$u_g = h_g - R_g T_i$ (for gas phase flow)

$u_l = h_l - \frac{p_{sat}}{\rho_w}$ (for liquid phase flow)

R_g = f(T_i, p_i, mass fraction of chemical specious in the gas phase)

ρ_w = f(T_i) p_{sat} = f(T_i)

(P_{sat}) is the saturation pressure and (ρ_w) is density at liquid water saturation.

The specific heat of the system is given by

$$c_{vsys} = \frac{d(m_g u_g)}{dT} + \frac{d(m_l u_l)}{dT} \tag{31}$$

which can be expand as

$$c_{vsys} = m_g \frac{du_g}{dT} + m_l \frac{du_l}{dT} + (u_l - u_g)\frac{dm_l}{dT} \tag{32}$$

Again, the first term in the right hand side of eq. 4.11 indicates the specific heat of the chemical species in the gas phase, the second term indicates the specific heat of liquid phase, and the last term indicates the rate of change of liquid to vapour phase, at constant volume.

$$c_{vsys} = \frac{U_2 - U_1}{T_2 - T_1} \tag{33}$$

where (U_2) is the internal energy at temperature (T_2) and (U_1) is the internal energy at temperature (T_1).

Density of a two phase flow system

The density of a system is defined as the mass per volume of the mixture and is given as:

$$\rho = \frac{m}{V} \tag{34}$$

The volume of the chemical species in the gas phase of the system is function of pressure, temperature and gas constant R_G, and gas phase composition.

V_g = f(p_i, T_i, R_G, gas phase composition) (35)

Also the volume of liquid phase is function of temperature and saturation pressure, i.e.

V_l = f(T_i) (36)

Thus the total volume of system is

$$V_{sys} = V_g + V_l \tag{37}$$

The density of the system per kg of mass is

$$\rho sys = \frac{1}{V_{sys}} \tag{38}$$

<u>sound velocity for a two phase flow system</u>

All the substances are compressible. The compressibility of any fluid id defined by the Bulk Modules of Elasticity denoted by (Ks) and is given by

$$Ks = \rho(\frac{dP}{d\rho}) \tag{39}$$

The sound velocity for the chemical specious of the gas phase in the system is

$$C = \sqrt{\gamma R g T i} = \sqrt{\frac{Kg}{\rho_g}} \tag{40}$$

where (g) denotes the chemical specious of gas phase in the system. Thus the bulk's modules of elasticity for the gas phase is given by

$$Kg = \rho_g \gamma R g T i \tag{41}$$

Hence the sound velocity of the system containing liquid water can be expressed as (Alan Vardy, 1990);

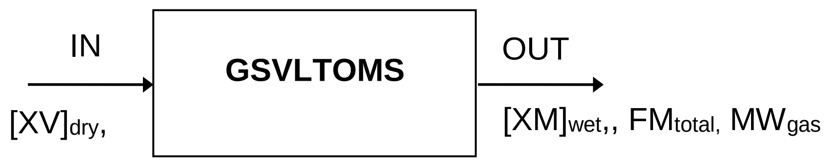
$$C_{sys} = \sqrt{\frac{\rho_g \gamma R g T i}{\rho sys}} \tag{42}$$

The speed of sound in a mixture containing liquid water is much smaller than the speed of gas phase alone. In a mixture containing liquid water, the compressibility factor is governed by the air whereas the density is governed by the water.

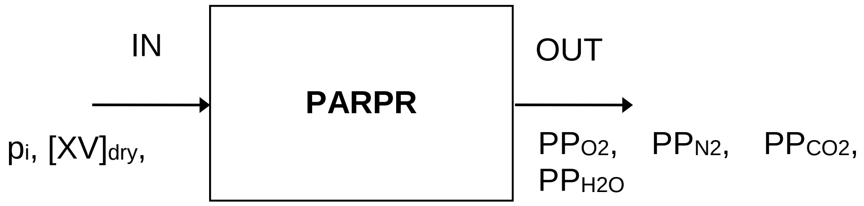
To show the fluid properties behaviour with different chemical composition and at various physical conditions, which may be encountered in practice, the following routines have been developed in the past to meet the necessity of having an inlet temperature ranging from -50°C to 60°C for various humidity conditions.

<u>VOLTMAFR</u> **<u>(volume to mass fraction routine)</u>** for a given ambient condition (i.e. dry volumetric compositions $[XV]_{dry}$, (consisting of O_2, N_2, CO_2, H_2O), relative humidity [φ], pressure [p_i], temperature [T_i]). This routine evaluates the mass fractions of the mixture $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, and H_2O).

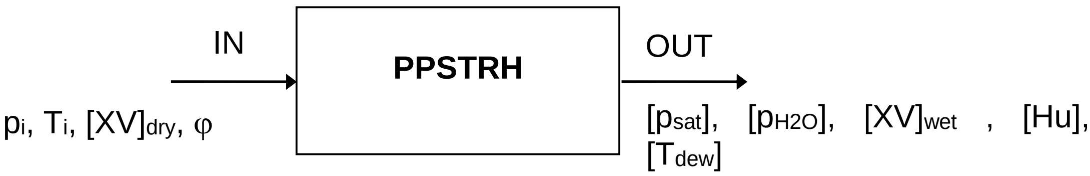
<u>GSVLTOMS</u> **<u>(gas volume to mass fraction)</u>** this routine evaluates the mass fractions of the mixture $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, H_2O), total mass fractions(FM_{total}) and gas molecular weight (MW_{gas}), for a given volumetric fractions of the mixture $[XV]_{dry}$, (consisting of O_2, N_2, CO_2, and H_2O).



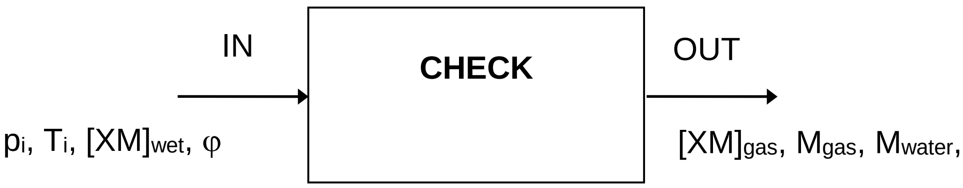
***PARPR* (partial pressure of the gas mixture)** this routine evaluates the partial pressure of different components in the mixture (i.e. PP_{O2}, PP_{N2}, PP_{CO2}, PP_{H2O},) for a given pressure(p_i), and volumetric fractions of the mixture $[XV]_{dry}$, (consisting of O_2, N_2, CO_2, H_2O).



PPSTRH given ambient condition (i.e. dry volumetric compositions $[XV]_{dry}$, (consisting of O_2, N_2, CO_2, and H_2O), relative humidity[φ], pressure [p_i], and temperature[T_i]). This routine evaluates the saturation pressure [p_{sat}], partial pressure of vapour [p_{H2O}], volumetric compositions of the mixture $[XV]_{wet}$ (consisting of O_2, N_2, CO_2, and H_2O), humidity ratio [Hu], and dew point temperature of the mixture [T_{dew}].

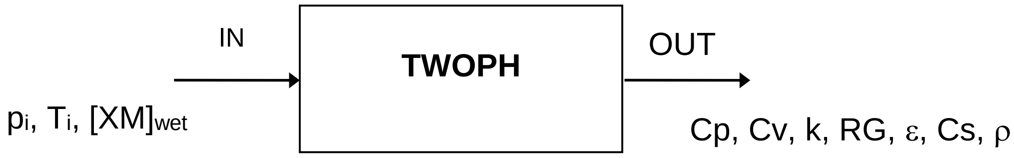


***CHECK* (subroutine check)** for a given pressure (p_i), temperature (T_i), and fractions of mass compositions in the mixture $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, and H_2O). This routine checks that the system is a mono-phase or two-phase flow. If there is a possibility of existence of water in the system, it calculates the amount of water in the system (M_{water}), total mass of chemical species in the gas phase of the system (M_{gas}), and gas mass fractions of each chemical species in the system (XM_{gas}).

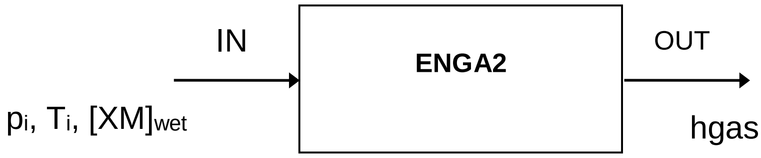


***GSTHPRM* (gas thermodynamic properties)** for a given pressure (p_i), temperature (T_i), and mass fractions of gas mixture $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, H_2O). This program is used to recognize the mixture condition (i.e. is it a mono-phase or two-phase flow). If it is a mono-phase flow, the routine calculates the mass of each chemical species in the gas phase. If there is a possibility of existing of liquid water, it calculate the mass of liquid water (M_{water}), and the mass fractions of each chemical species in the gas phase of the system (XM_{gas}). In addition the routine calculate the thermodynamic quantities of the mixture (i.e. specific heat at constant. pressure [Cp], specific heat at constant volume [Cv], gas constant[RG], specific heat ratio of the system [k], polytropic exponent of the mixture [ε], sound velocity [Cs], and density of the gas mixture for the-mono phase flow or two-phase flow [ρ].

***TWOPH* (two phase flow)** for a given pressure(p_i), temperature(T_i), and fractions of wet mass compositions in the gas mixture $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, H_2O). This routine obtains the thermodynamic properties of the mixture, when some amount of water exists in the mixture (i.e. specific heat at constant pressure[Cp], specific heat at constant volume [Cv], specific heat ratio of the system [k], polytropic exponent of the wet mixture [ε], density of the mixture [ρ], and sound velocity [Cs]).

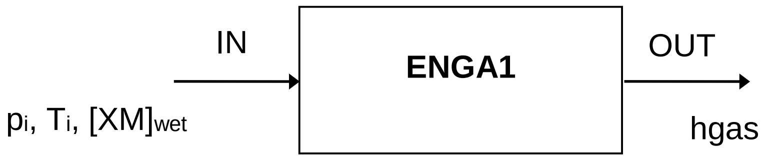


***ENGA2* (enthalpy of gas mixture)** this routine calculate the specific enthalpy of gas phase mixture for a given pressure (p_i), temperature (T_i), and fractions of compositions $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, H_2O). In this routine the heat of vaporization of water vapour is not considered.



***HGA2* (gas enthalpy)** calculate the specific enthalpy of a gas mixture for a given temperature (T_i), and mass fraction of compositions $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, H_2O). In this routine the heat of vaporization of water vapour is not considered.

***ENGA1* (enthalpy of gas mixture)** this routine calculate the specific enthalpy of gas phase mixture for a given pressure (p_i), temperature (T_i), and fractions of compositions $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, H_2O). In this routine the heat of vaporization of water vapour is being considered.



***HGA1* (gas enthalpy)** calculates the specific enthalpy of a gas mixture for a given temperature (T_i), and mass fraction of compositions $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, H_2O). In this subroutine the heat of vaporization of water vapour is being considered.

GASCO for a given air compositions $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, H_2O), fuel constituents $[XM]_{fuel}$ (consisting of C, H_2, O_2, N_2, S, H_2O), and air-fuel ratio (α).
This routine determines

1. fractions of gas products at combustion chamber exit for burning 1 kg of fuel $[XM]_{wet}$ (consisting of O_2, N_2, CO_2, H_2O).
2. stoichiometric air-fuel ratio, and
3. percentage of excess air.

SPHTG calculate the specific heat of the gas phase at constant pressure for a given gas temperature and gas compositions (consisting of O_2, N_2, CO_2, and H_2O).

Accordingly, computer programmes have been written for each of the above cases, incorporating correlations for calculating the gas properties, by implementing the concepts discussed above. Moreover, already existing water steam thermodynamic functions have been improved to have a shorter computing time. Modifications to traditional subroutines have been introduced, to have an exact matching of enthalpy values (and of other quantities) on both saturated water and saturated steam lines when such quantities are calculated with functions valid in two adjoining regions. In order to calculate the thermodynamic quantities below the triple point, properties of solid phase and solid-vapour mixture phase have been added to the routines.

Component Models: an example

As described in the previous paragraphs, each component can be schematized as a black box. It exchanges with the other plant components input and output quantities and it is characterized by some attributes. In a lot of design problems, where a large number of variables are involved, the use of dimensional analysis is of great interest to search the machine arrangements which can address the best performance. In other cases, detailed thermodynamic and fluid dynamic models are more useful to describe the component behaviour. In the following paragraph some models for axial and radial compressors available at RO3 are described. All the other components presented in the list above are organized following the same philosophies.

Compressors (Axial and Radial)
The model uses the following equations:

- mass conservation

$$\rho_j A_j w_j \sin\beta_j - \rho_{j+1} A_{j+1} w_{j+1} \sin\beta_{j+1} = 0 \qquad (43)$$

ρ is the density, (A) is the annular section, (β) and (ω) are the fluid angle and blade relative velocity.

- energy conservation

$$h_{j+1} + 1/2\cdot(w_{j+1}^2 - u_{j+1}^2) = h_j + 1/2\cdot(w_j^2 - u_j^2) \qquad (44)$$

(h) and (u) represents the enthalpy and blade velocity.

- Momentum conservation

The work done by the rotor on the fluid, from the steady flow energy equation and momentum equation is:

$$L_E = u_{j+1} w_{j+1} \cos\beta_{j+1} - u_j w_j \cos\beta_j + u_{j+1}^2 - u_j^2 \qquad (45)$$

- <u>Correlation for the calculation of the losses</u>

The total pressure losses in cascade is obtained with respect to the isentropic transformation. The total pressure at exit is correlated with the fluid condition at inlet;

$$p^0_{r,j+1} = p_j\left(\frac{T^0_{r,j}}{T_j}\right)^{cp/R} - \frac{1}{2}\rho_j w_j^2 \omega \qquad (46)$$

where (T^0_r) is the total cascade temperature obtained from the conservation of energy given in equation 44:

$$T^0_r = T_j + \frac{w_j^2 - u_j^2}{2cp} \qquad (47)$$

(ω) being the global coefficient of the total pressure loss defined as:

$$\omega = \frac{\Delta p^0_r}{\frac{1}{2}\rho_j w_j^2} \qquad (48)$$

The relation (48) is a generalized form of equation for the rotor and stator. In this equation the velocity corresponds to the relative velocity in rotor and absolute velocity in the stator. Of course, the relative velocity of the stator blade is zero.
The model contains other relations that furnish thermodynamic properties.
The compression process for the complete stage is presented on a Mollier diagram in fig. 10, which is generalized to include the effect of irreversibility.

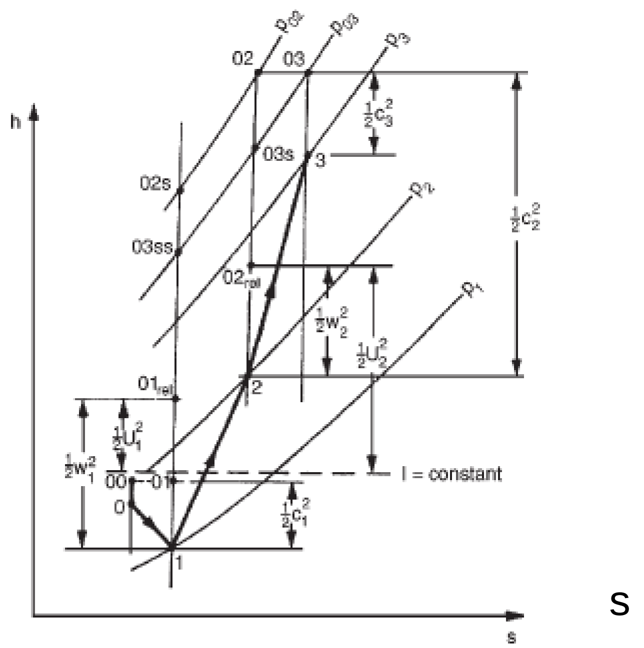


Figure 10: Mollier diagram for the complete centrifugal compressor stage

<u>Model for Cycle calculation</u>

The correlation adopted to calculate the compression process is expressed by thermodynamic differential equation,

$$\frac{dT}{T} = \frac{k-1}{k}\cdot\frac{1}{\eta_p}\cdot\frac{dp}{p} \qquad (49)$$

with (dp) being polytropic efficiency, (k) ratio of specific heats which is calculated as a function of pressure, temperature, and gas compositions.
Calculation across compressor is conducted by dividing compressor inlet and exit pressure into small intervals (nint) of equal segments.
Given the compressor inlet conditions (i.e. inlet pressure, temperature and air mass flow) and exit pressure, and assuming compressor exit temperature (the exit temperature may be assumed equal to the inlet temperature), the actual compressor exit temperature can be obtained iteratively by integrating the polytropic transformation given in eq. 49, i.e.

$$\frac{T_{u,j}}{T_{i,j}} = \left(\frac{p_{u,j}}{p_{i,j}}\right)^{\frac{k_j-1}{k_j}\cdot\frac{1}{\eta_p}} \tag{50}$$

(Ti,j) and (Tu,j) respectively are the temperatures at inlet and exit of each interval j-th, (pu,j) and (pi,j)are the corresponding pressures, and (kj) represents the specific heat ratio correspond to the inlet condition. The calculation is performed simultaneously. The exit conditions from one interval are the inlet conditions to the next interval.

<u>Sizing</u>
As mentioned before, the models are based on a Finite Volume row-by-row lumped concept. For example, the through flow scheme for an axial compressor is shown in figure 2.
The model is used to solve the inverse problem which determines the geometry and global parameters to characterize the compressor.
Figure 11 represents a cascade to cascade geometry flow for an axial machine, considering the following equations written for the j^{th} and $j+1^{th}$ station with respect to inlet and exit to each cascade.
The aim of the sizing procedure is having a component equivalent to the real one whose real size are not known and there are not enough information (from the manufacturer).
The geometry data of compressor are provided by the manufacturer. If these data are not available they are calculated by a preliminary solution of an inverse (sizing) problem using RO3 methodology.
The empirical models of the flow features and performance reported in this section is one of the option that can be chosen according to the machine type.
Some quantities at nominal conditions are given as inputs. For example, for an axial compressor they are:

- air mass flow; kg/s
- rotational speed; rpm
- inlet pressure (p_{in}); bar
- inlet temperature (T_{in}); °C
- pressure ratio (β);
- number of stages (N_{stage});
- number of stator with varying geometry;
- inlet air mass compositions; %
- index for the presence of inlet and outlet guide vanes [VIGV and OGV]; (if 0 there is no VIGV, if 1 There exists an VIGV).
- index for velocity; (if 0 then speed is constant, if 1 speed is varying, then the program read the maximum and minimum velocities);
- constructive efficiency;
- optimum reaction coefficient;
- maximum peripheral velocity ($u1_{max}$);
- maximum Mach number (Ma_{max});
- design total exit temperature ($t3_{des}$).

Variables introduce in the program are:

- blade heights for each station (i.e. stator and rotor);
- peripheral blade velocity (u_1) corresponding to the 1st station;
- ratio of actual losses to that of calculated losses (fr).

Geometrical quantities are unknowns.

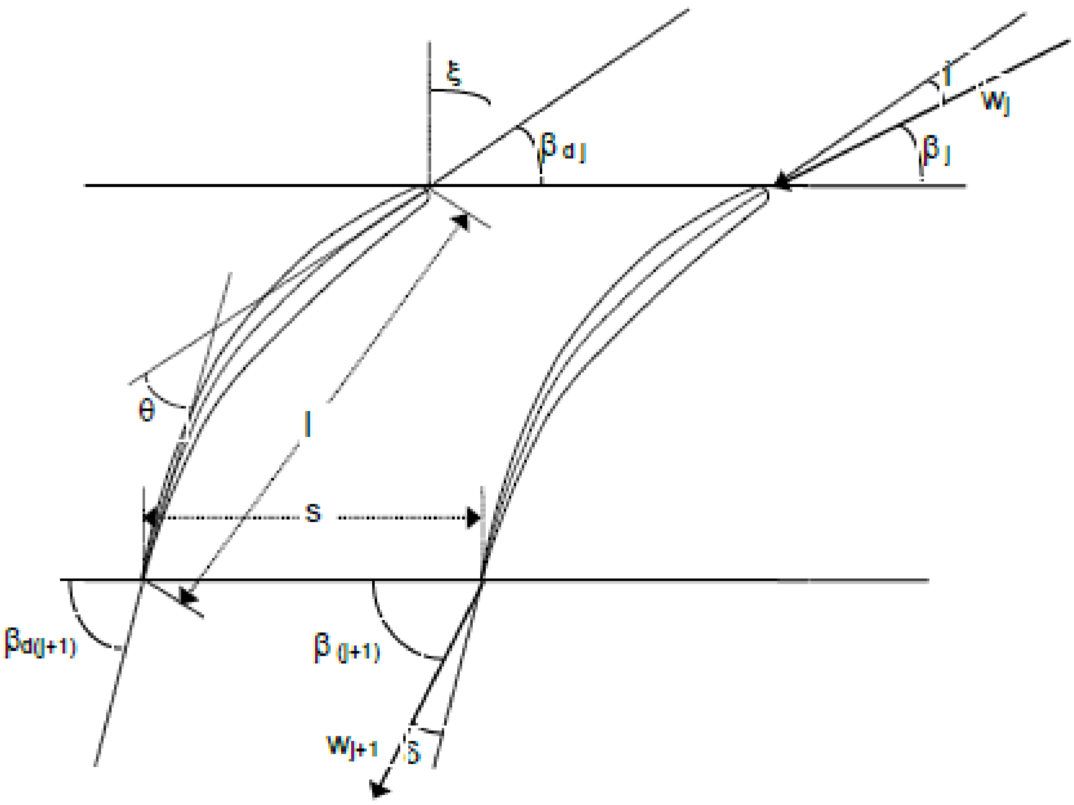


Figure 11: Nomenclature adopted for a cascade (axial compressor)

The compressor model calculates thermodynamic and fluid dynamic quantities at the exit of each row (which are the entrance to the next row), the whole machine calculate the stacking of the contribution of various rows. The model use mass, energy, continuity, and 2nd law equation, empirical correlations for losses, and deviation calculations.

Consider one stage of the compressor consisting of a fixed and moving row (i.e. stator and rotor). The inlet flow to the first row (stator or VIGV) is indicated by station 1. The exit quantities from first row which are the inlet quantities to the next row is denoted be station 2, and the exit of moving row is shown by station 3.

The thermodynamic quantities and geometric data using row-by-row sizing of the compressor are obtained from the following relations.

First of all, experience has indicated that the axial velocity should remain constant at the design point. Thus

$$w_j \sin\beta_j - w_{j+1} \cos\beta_{j+1} = 0 \quad (50)$$

and

$$C_j \sin\alpha_j - C_{j+1} \sin\alpha_{j+1} = 0 \quad (51)$$

(w_j) and (w_{j+1}) being the relative velocities at inlet and exit. (Cj) and (Cj+1) are the absolute velocities. (α) and (β) are the relative and absolute angles as shown in the triangular velocity diagram (see fig. 12).

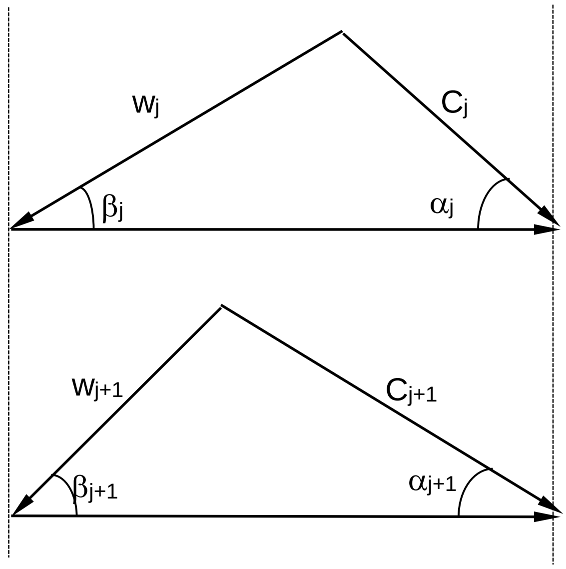


Figure12: Axial flow compressor velocity diagrams

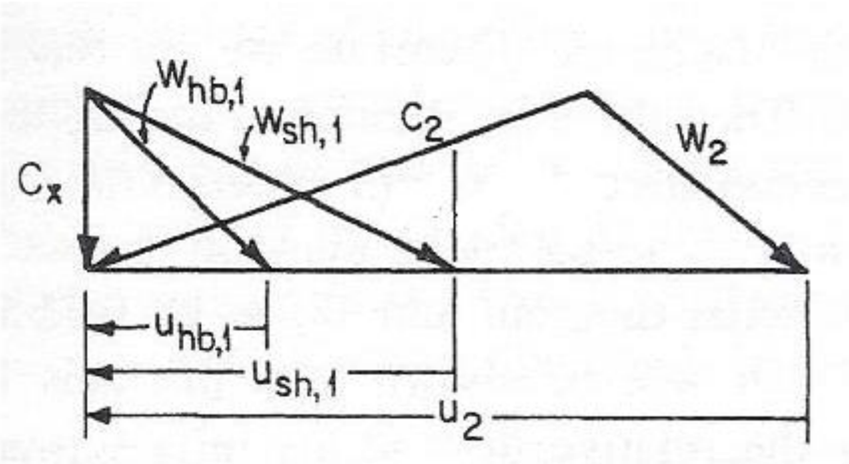


Figure 13: Radial flow compressor velocity diagrams

Total and static temperatures and pressures

The static temperature at the rotor inlet is

$$T_j = T_{in} - \frac{C_j^{\,2}}{2C_p} \qquad (52)$$

The static pressure at the rotor inlet is

$$p_j = p_{in}\left(\frac{T_j}{T_{in}}\right)^{Cp/R} \qquad (53)$$

The total relative temperature at the rotor inlet is

$$T^{\circ}_{rj} = T_j + \frac{w_j^{\,2} - u_j^{\,2}}{2C_p} \qquad (54)$$

The relative total pressure is

$$p^{\circ}_{rj} = p_j\left(\frac{T^{\circ}_{rj}}{T_j}\right)^{Cp/R} \qquad (55)$$

The total relative temperature at the rotor exit is equal to that of the rotor inlet, therefore, the static temperature is given by

$$T_{j+1} = T^{\circ}_{rj} - \frac{w_{j+1}^{2} - u_{j+1}^{2}}{2C_p} \qquad (56)$$

Losses are taken into account. For a radial machine, they are due to:

- Incidence;
- Skin Friction;
- Diffusion and blade loading;
- Clearance;
- Shock wave;
- Disk friction;
- Secondary effects.

Empirical correlations are used to evaluate such losses for each kind of machine.

Part load analysis

The schematic diagram of the model is shown in figure 14.

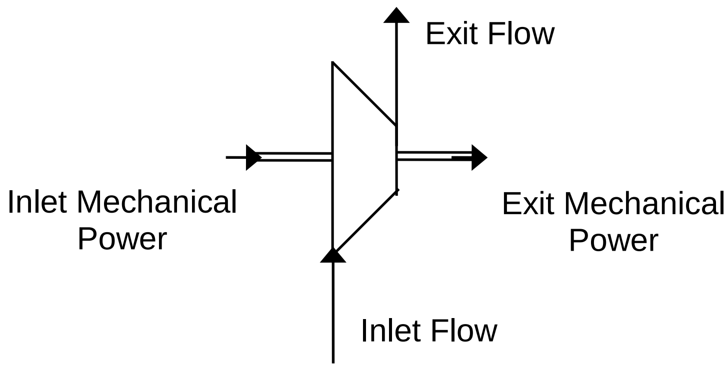


Fig.14: Schematic model of axial compressors

The corresponding inlet and exit variables and power across the compressor are defined as:

Inlet: mass flow, pressure, temperature, composition (mass fractions)
Exit: mass flow, pressure, temperature, composition (mass fractions)
Inlet mechanical power: mechanical power, rotational speed

Compressor geometric data are given as inputs. For example for an axial stage:

- VIGV absolute flow angles at inlet and exit, camber angle, solidity (of course these quantities are read if VIGV exists);
- stator absolute angles at inlet and exit;
- rotor relative angles at inlet and exit;
- diameter ratios;
- height at each station;
- area at each station;
- stator and rotor camber angles;
- stator and rotor stagger angles;
- stator and rotor solidity;
- stator and rotor aspect ratio;
- stator and rotor maximum thickness ratio;
- stator and rotor pressure losses;

- stator and rotor inlet and exit blade angles;
- stator and rotor incidence angle;

The different operating points are determined giving the values of:

- compressor inlet pressure and temperature;
- rotational speed;

For the off-design condition the following relations are used:

$$F(\beta,m,t_i,p_i,n,\alpha) = 0 \tag{57}$$

and

$$F(\beta,\eta,t_i,p_i,n,\alpha) = 0 \tag{58}$$

Being (p_i) and (T_i) the inlet conditions to the compressor, $\beta=p_u/p_i$ the compressor pressure ratio, η the adiabatic efficiency. (n) is the rotational velocity and (α) is the parameter for the opening of the VIGV for stator cascade with variable geometry.
For each value of the parameters (n) and (α) the calculation is done for different machine fluid inlet temperature. The user gives maximum and minimum values of the temperature.
On each curve surge condition is assumed when the row is stalled. Stall limits for positive and negative incidence angle are found using empirical diagrams.

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Component Models available at University of Seville

The currently available models for are briefly introduced in the next paragraphs. Furthermore, main characteristics and some preliminary results are presented.

The simulator of the OMSoP system comprises a series of lumped-volume models that describe the behaviour of every component, thus simulating its physical functioning with a sequential resolution of the governing equations. The structure of the complete model is:

- Preliminary evaluation of the cycle performance and sensitivity analysis of the main dependent variables with respect to the global parameters that define the quality of the components at design conditions.
- Design of the main components in rated conditions. This process uses technical information gathered from literature (public domain) for similar apparatus, governing equations based on the physical behaviour of each piece of equipment and empirical relations to evaluate the different losses. The individual off-design maps and the matching amongst the components are calculated in this phase.
- Steady-state performance evaluation of the cycle in off-design operation. Different operating strategies can be imposed.

<u>Reference hot air recuperative Brayton cycle</u>

The simulator developed at the University of Seville is based on an engine working on a recuperative Brayton cycle running on hot air. A list of components follows:

- Single stage centrifugal compressor;
- Flat plate recuperator;
- Radial in-flow turbine, driving the compressor and generator in a single shaft arrangement.
- Electric generator and inverter to allow for variable speed electricity production.
- Pressurised volumetric receiver between compressor and turbine. The model considered for this component has been taken from previous works by KTH
- Parabolic dish concentrator.

This model is used to predict the annual production of electricity (yield) of the system and to calculate the LCOE and NPV with various economic and financial conditions. A sample plot of the solar-to-electricity efficiency of the system in on and off-design operation is presented below as a function of the available insolation. It is worth noting that the thermo physical properties of the working fluid have been evaluated considering the air as ideal gas.
The previous result is valid for the solar-only system and thus a different evaluation will have to be produced for the hybrid configuration to account for various operating strategies.

The simulation has been implemented in Matlab environment and will be later used in a genetic algorithm structure to optimise the system from technical and economic standpoints. To this aim, the objective cost function will be implemented based on real data.

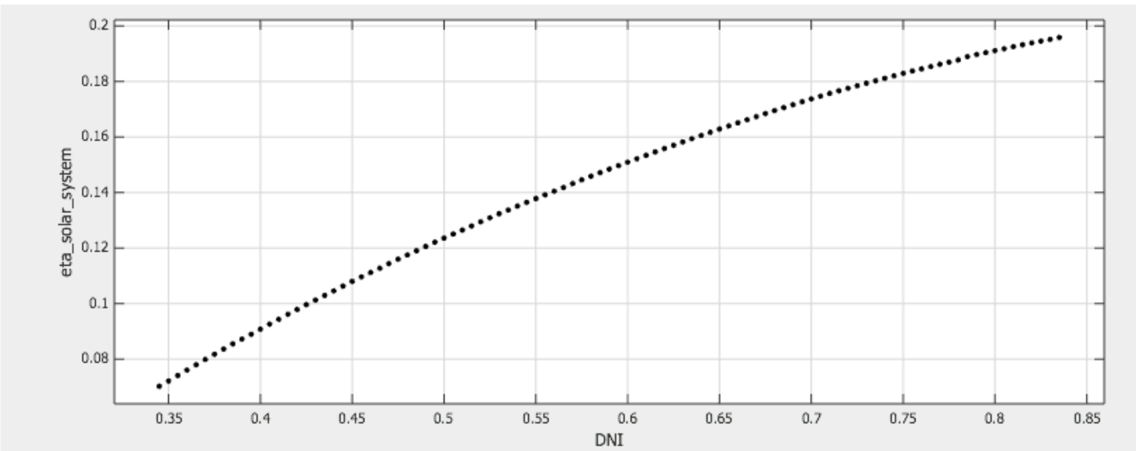


Fig.15: Calculated overall system efficiency VS Direct Normal Irradiance (DNI)

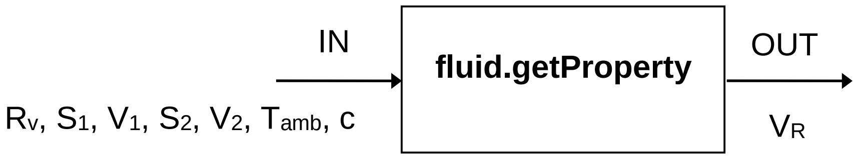
The simulation of the system will expectedly be improved with other models available in the consortium to compare different systems layout.

List of KTH models
The list below shows the models available at KTH and developed on its own.

- Fluid Properties
- Compressor
- Recuperator/Heat Exchanger (design condition)
- Recuperator/Heat Exchanger (off-design condition)
- Solar receiver (design condition)
- Solar receiver (off-design condition)
- Combustor
- Turbine
- Solar Receiver Design
    - 1D for different types
    - 2D-axisymmetric for different types
    - 3D for different types
- Thermoeconomic Model

Description of the models

Fluid Properties
Fluid properties for air, water and combustion gases are taken from the NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP) and accessed via a MATLAB routine and a MATLAB Executable (MEX).

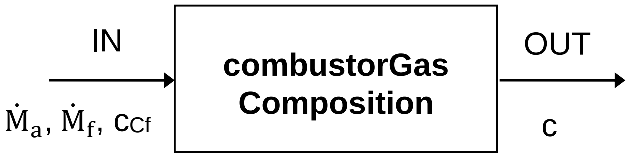


Obtain the value V_R of the fluid property specified in R_v, at the point specified by the values of the properties S_1 and S_2. The inputs V_1 and V_2 can be scalars or vectors. T_{amb} is necessary only for calculation of the co-enthalpy. For acquiring properties of combustion gases the gas composition c needs to be specified. Properties are calculated using the refpropm routine developed by NIST (see: help refpropm). The viable character strings are:

Abbreviation	Name	Unit
P	Pressure	Pa
T	Temperature	K
D	Density	kg/m³
H	Enthalpy	J/kg
U	Internal energy	J/kg
Q	Quality	kg/kg
S	Entropy	J/kg
C	Specific heat capacity c_p	J/kgK
O	Specific heat capcity c_v	J/kgK
K	Co-Enthalpy	J/kg
V	Dynamic viscosity	Pa s
L	Thermal conductivity	W/mK
A	Speed of sound	m/s
I	Surface tension	N/m

S_1 must be chosen from amongst: T P H D
S_2 must be chosen from amongst: P D H S U Q

The gas composition c can be determined using an additional model. The input variables $\dot{\mathrm{M}}_{\mathrm{a}}$ and $\dot{\mathrm{M}}_{\mathrm{f}}$ denote the mass flow of air and fuel respectively, whereas c_{Cf} is the carbon content of the fuel.



The output variable c is a vector containing the mass percentage of the following gases.

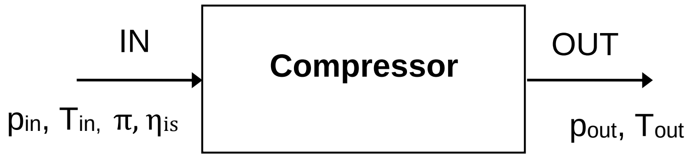
- Nitrogen N_2
- Oxygen O_2
- Argon Ar
- Carbon dioxide CO_2
- Water vapour H_2O

<u>Micro Gas-Turbine Component Models (Design Condition)</u>

The component models of the gas-turbine cycle for the design condition are based on standard equations and the fluid property models described above.

<u>Compressor:</u>

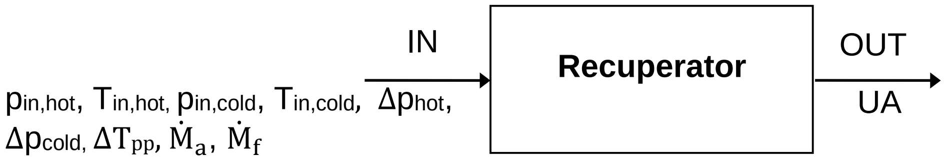
The outlet temperature is a determined using the fluid property model explained above based on the outlet enthalpy h_{out}.



Input variables are the pressure p_{in}, the temperature T_{in}, the compressor pressure ratio π, and the isentropic efficiency η_{is}. Outlet variables are the pressure p_{out} and the temperature T_{out}.

<u>Recuperator:</u>

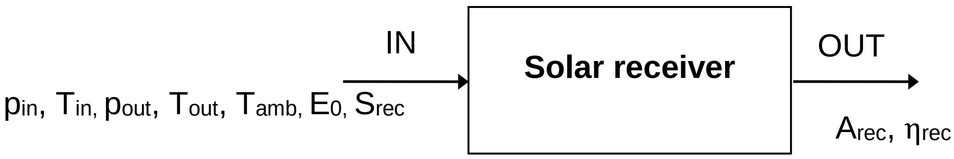
The needed overall heat transfer coefficient UA of the recuperator for a given power cycle is determined based on the NTU method [1] and the fluid property model explained above.



Input variables are the inlet pressure p_{in}, and the inlet temperature T_{in}, of both the hot and cold side of the recuperator. Δp the pressure drop in the hot and cold side and ΔT_{pp} is the temperature difference at the pinch point. Moreover, the $\dot{M}_a$ and $\dot{M}_f$ denote the mass flow of air and fuel respectively.
Output variable is the overall heat transfer coefficient UA.

<u>Solar receiver:</u>

A simple model of a solar receiver is used to calculate the receiver size for a given power cycle.



Input variables are the inlet and outlet pressure p and temperature T, the ambient temperature, the solar flux at the aperture, and the following receiver specifications

- Absorptivity of the absorber
- Convective heat transfer coefficient to the ambient
- Transmissivity of the glass window (depending on the type)
- Optical efficiency of a secondary compound parabolic concentrator (CPC)

As an output variable the receiver area A_{rec} and efficiency η_{rec} are calculated using heat balances and the fluid property model described above.

Combustor:
The specific fuel consumption is calculated based on the fluid property model describe above.

p_{in} , T_{in}, Δp, T_{out}, , Δp, c_{Cf} $\xrightarrow{\text{IN}}$ **Combustor** $\xrightarrow{\text{OUT}}$ $\dot{m}_f$

Input variables are the inlet pressure p_{in}, and the inlet temperature T_{in}, as well as the desired outlet temperature T_{out} and the pressure drop Δp. The variable c_{cf} denotes the carbon content of the fuel burnt. Output variable is the specific fuel consumption.

Turbine:
The outlet temperature is a determined using the fluid property model explained above based on the outlet enthalpy h_{out}.

p_{in}, T_{in}, p_{out}, η_{is} $\xrightarrow{\text{IN}}$ **Turbine** $\xrightarrow{\text{OUT}}$ T_{out}

Input variables are the inlet and outlet pressure p_{in} and p_{out}, the inlet temperature T_{in}, and the isentropic efficiency η_{is}. Outlet variable is the outlet temperature T_{out}.

Micro Gas-Turbine Component Models (Off-Design Condition)
The component models of the gas-turbine cycle for the off-design conditions (yearly calculation) differ slightly from the design-condition models. However, they are also based on standard equations and the fluid property models described above.

Recuperator:
The outlet temperature is a determined based on the NTU method [1] and the fluid property model explained above.

$p_{in,hot}$, $T_{in,hot}$, $p_{in,cold}$, $T_{in,cold}$, $\dot{M}_a$, $\dot{M}_f$, UA, Δp_{hot}, Δp_{cold} $\xrightarrow{\text{IN}}$ **Recuperator** $\xrightarrow{\text{OUT}}$ $p_{out,hot}$, $T_{out,hot}$, $p_{out,cold}$, $T_{out,cold}$

Input variables are the inlet pressure p_{in}, and the inlet temperature T_{in}, of both the hot and cold side of the recuperator. Moreover, the $\dot{M}_a$ and $\dot{M}_f$ denote the mass flow of air and fuel respectively. UA is the overall heat transfer coefficient, and Δp the pressure drop in the hot and cold side.
Output variables are the outlet pressure p_{out}, and the outlet temperature T_{out}, of both the hot and cold side of the recuperator.

Solar receiver:
A simple model of a solar receiver is used to calculate the outlet temperature for a given receiver (given area).

p_{in}, T_{in}, p_{out}, T_{amb}, E_0, S_{rec} $\xrightarrow{\text{IN}}$ **Solar receiver** $\xrightarrow{\text{OUT}}$ T_{out}, η_{rec}

Input variables are the inlet and outlet pressure p and the inlet temperature T, the ambient temperature, the solar flux at the aperture, and the following receiver specifications

- Solar receiver area

- Absorptivity of the absorber
- Convective heat transfer coefficient to the ambient
- Transmissivity of the glass window (depending on the type)
- Optical efficiency of a secondary compound parabolic concentrator (CPC)

As an output variable the outlet temperature T_{out} and the efficiency η_{rec} are calculated using heat balances and the fluid property model described above.

<u>Solar Receiver Models</u>

For more detailed solar receiver designs different model of different complexity are available.

<u>1D model</u>

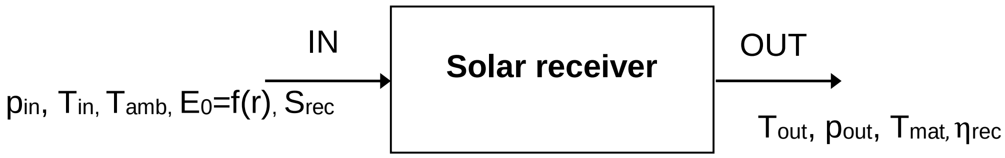
As described above.

<u>2D-axisymmetric model (MATLAB)</u>

This model is based on MATLAB routines using a finite volume scheme to determine the material and fluid temperatures as well as the pressure drop within the receiver. A detailed description is provided in a journal publication [2].

Input variables are the inlet pressure p and the inlet temperature T, the ambient temperature, the solar flux at the aperture (as a function of the radius), and the receiver specifications including

- Solar receiver geometry
- Absorptivity of the absorber
- Convective heat transfer coefficient to the ambient
- Transmissivity of the glass window (depending on the design)
- Optical efficiency of a secondary compound parabolic concentrator (CPC)



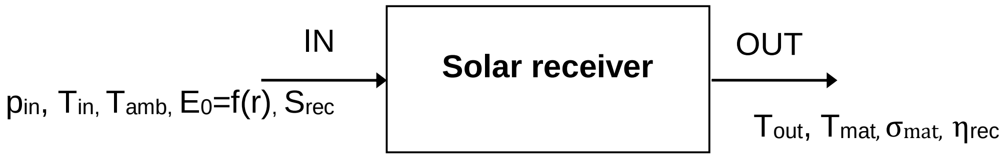
As an output variable the outlet temperature T_{out}, the outlet pressure p_{out}, the material temperatures T_{mat}, and the efficiency η_{rec} are calculated using the local thermal non-equilibrium model and the fluid property model described above.

<u>2D-axisymmetric model (MATLAB+COMSOL)</u>

This model is based on a coupled MATLAB and COMSOL approach using a coupled CFD/FEM analysis to determine the material and fluid temperatures, material stresses, as well as the pressure drop within the receiver. A detailed description is provided in a journal publication [2].

Input variables are the inlet pressure p and the inlet temperature T, the ambient temperature, the solar flux at the aperture (as a function of the radius), and the receiver specifications including

- Solar receiver geometry
- Solar receiver materials
- Absorptivity of the absorber
- Convective heat transfer coefficient to the ambient
- Transmissivity of the glass window (depending on the design)
- Optical efficiency of a secondary compound parabolic concentrator (CPC)



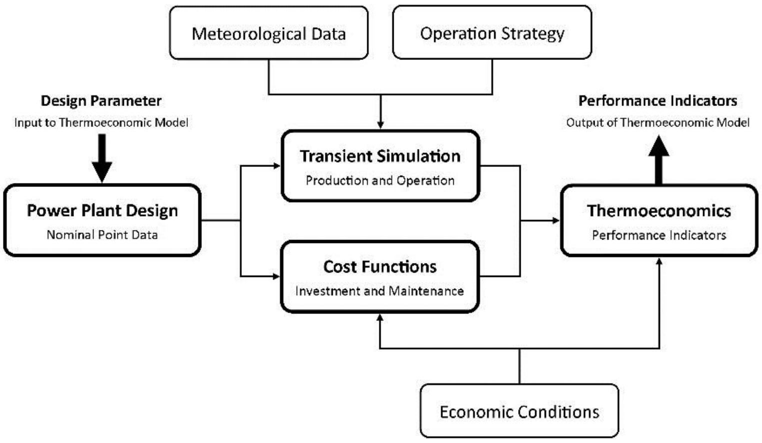
As an output variable the outlet temperature T_{out}, the outlet pressure p_{out}, the material temperatures T_{mat} and stresses σ_{mat}, and the efficiency η_{rec} are calculated.

<u>3D model (FRED+FLUENT)</u>

For a fully 3 dimensional analysis the results of the ray-tracing software FRED are used as an input for a CFD analysis of a solar receiver in ANSYS FLUENT.
The model uses the same input values as the 2D-axisymmetric model with the addition that a three-dimensional flux profile is used $E_0 = f(r,x)$.

Thermoeconomic models

In order to design hybrid solar MGT power plants and evaluate their performance, a thermoeconomic model, which combines thermodynamic performance calculations with cost predictions, has been developed. A flow sheet of the thermoeconomic model is shown below.



The first segment of the model calculates the nominal design of the system and the size of the different components. The equipment sizes and nominal point data are then sent to the transient calculation which determines the off-design performance of the system; in order to account for the high variability of the solar resource, annual simulation is essential to obtain a representative evaluation. The nominal power plant design is also used to calculate the capital cost of the power plant equipment. These cost figures can then be combined with the annual performance data (mainly the annual fuel consumption) and additional economic data to calculate the total investment and operating costs. At the end of the thermoeconomic analysis a series of relevant performance indicators, such as equivalent annual costs and carbon dioxide emissions can be calculated. A detailed description is given in the PhD thesis of Spelling [3].

KTH References

[1] T. Bergman, A. Lavine, F. Incropera et al., 2011, Fundamentals of Heat and Mass Transfer, Seventh Edition, John Wiley & Sons, Inc.
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Models available at City University

City University is working on a model for simulating the whole engine (MGT) which at the end will be able to do the following stages:

- Design point calculation which will give engine configuration, component size, compressor pressure ratio, mass flow rate, fuel/air ratio (in case of combustion), turbine inlet temperature (or turbine exit temperature), pressure drops, expected efficiencies for components and the whole engine and rotational speed;
- Evaluation of the off-design and part load behaviour;
- Optimisation of the engine design.

The model is considered to be in 0-D level which means that it will use available or scaled performance maps for the components or applies the lumped model calculations.

<u>Simple cycle analysis for gas turbine</u>

To study the thermodynamic cycle performance of the gas turbine in OMSoP project, a simple analysis has been made. The formulation is based on an open cycle, single-shaft gas turbine including a heat exchanger (recuperator) which uses the exhaust gas from the turbine to pre-heat the compressed air leaving the compressor. To make the calculation easier when investigating the influence of cycle parameters, a FORTRAN program has been created which is considered as the main platform for future optimisation of the cycle. The results show the prominence of Turbine Inlet Temperature (TIT) and compressor ratio as well as other factors like pressure drop along the circuit and efficiencies of components, mainly; turbine, compressor and recuperator.

Thermodynamic cycle

The thermodynamic cycle of a single shaft heat exchanged simple gas turbine is shown if Fig. 1.

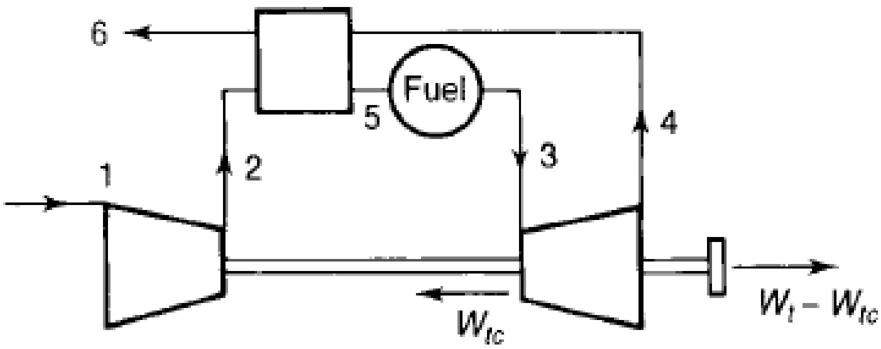

Fig. 16 Simple heat exchanged gas turbine cycle

Cycle calculation

Some of the working conditions are known (or can be assumed as known) which are ambient temperature and pressure (T_{amb}, p_{amb}) and maximum temperature in the circuit i.e. Turbine Inlet Temperature (TIT). The latter is normally limited by material considerations or project specification. Other information for the components is assumed based on the expected normal performances of the components which were available in technical literature or suggested by project contributors. These are mass flow rate ($\dot{m}$), efficiencies of the turbomachinery, electric generator, effectiveness of the recuperator etc. so is pressure drop across the circuit which is normally expressed related to the inlet pressure of each section (*dp/p*).

Thermodynamic relations

Compressor stagnation conditions at the inlet can be considered as equal to the ambient conditions:

$T_{01} = T_{amb}$

$p_{01} = p_{amb}$

Then:

$p_{02} = r \times p_{01}$

$p_{05} = p_{02} - \frac{dp}{p_{02}}$, $p_{03} = p_{05} - \frac{dp}{p_{05}}$, $p_{06} = p_{04} - \frac{dp}{p_{04}}$

If the outlet gas is directly exhausted to the surroundings, then $p_{06} = p_{amb}$.
Isentropic temperature rise due to compression:

$T_{02s} = T_{01}\left(\frac{p_{02}}{p_{01}}\right)^{(\gamma-1)/\gamma}$, $T_{04s} = T_{03}\left(\frac{p_{04}}{p_{03}}\right)^{(\gamma_g-1)/\gamma_g}$

Based on the definition of isentropic efficiency for compressor and turbine:

$T_{02} = T_{01} + \frac{(T_{02s}-T_{01})}{\eta_c}$, $T_{04} = T_{03} - \eta_t(T_{03} - T_{04s})$

For recuperator:

$\eta_{rec} = \frac{T_{05}-T_{02}}{T_{04}-T_{02}}$, $T_{05} = T_{02} + \eta_{rec}(T_{04} - T_{02})$

Now it is possible to calculate works of the compressor and turbine and also the virtual heat input by combustion in the burner.

$w_c = C_p(T_{02} - T_{01})$, $w_t = C_{pg}(T_{04} - T_{03})$

$w_{Net} = w_t - w_c$

$q_H = C_{pg}(T_{05} - T_{03})$

In case of having combustion in the burner, calculations must be done for the combustion considering the type of fuel and combustion efficiency in the burner. It is also important to consider properties of the combustion products in the burner and after that. So, the related equations must be corrected.

$w_t = C_{pg}(T_{04} - T_{03})$, $q_H = C_{pg}(T_{05} - T_{03})$, $T_{04s} = T_{03}\left(\frac{p_{04}}{p_{03}}\right)^{(\gamma_g-1)/\gamma_g}$

Based on the inlet temperature and temperature rise in the burner, fuel air ratio “f” can be derived from reaction heat. Specific Fuel Consumption (SFC) can then be found as

$$SFC = \frac{f}{w_{Net}}$$

Cycle efficiency based on fuel SFC would be:

$$\eta = \frac{w_{Net}}{f \times Q}$$

Where Q is calorific value of the fuel
This may be slightly different from the basic thermal efficiency of the cycle as:

$$\eta_{th} = \frac{w_{Net}}{q_H}$$

List of component models

At the moment, City has the following modules:

- Compressor and Turbine:
  Input: raw data collected from digitised maps.
  Output: specifications of automatically selected reference point, normalised non-dimensional data for pressure ratio, mass flow rate and efficiency, scaled (fitted) map.
- Combustor
  Input: type (composition of the fuel), inlet temperature, inlet pressure, outlet temperature, air mass flow rate
  Output: fuel/air ratio, fuel mass flow rate,
- Recuperator
  Input: mass flow rate (hot and cold sides), inlet pressures and temperatures (hot and cold sides), dimensional data (size)
  Output: outlet pressures and temperatures (hot and cold sides)

City is, also, working on the development of the following modules:

- High Speed Generator, model will determine HSG's output against absorbed torque etc.
- Oil system, this is needed to account for losses that we may have in the system
- A model to account for the mechanical losses in the shaft and bearing and/or windage

Program input, output and attributes

- Inputs:
  - Tabulated data for compressor and turbine (extracted points from the digitised performance maps). For any particular point these data include corresponding pressure ratio, mass flow rate, isentropic efficiency, and speed. Overall sizes of compressor and turbine are also needed as the input;
  - Other components data: recuperator efficiency (effectiveness) and flow-pressure drop characteristics for the recuperator and combustor (receiver) pressure drop characteristics.
  - Ambient condition (pressure and temperature) and exit flow total pressure.
  - Working conditions: output power required and limitations to maximum turbine temperature (inlet or exit).
  - Fluid properties: humidity (will be added later) and composition of the fuel (when model is run considering combustion).
  - Initial guess for the main unknowns (compressor's non-dimensional speed and pressure ratio, fuel air ratio, compressor exit temperature, turbine's inlet and exit temperature, turbine pressure ratio and exit pressure and turbine's non-dimensional speed.

- Outputs:
  - Temperature and pressure values at all stations (inlet and outlet of gas turbine's components).
  - Output power.
  - Calculated working point data: compressor's non-dimensional speed and pressure ratio, fuel air ratio, compressor exit temperature, turbine's inlet and exit temperature, turbine pressure ratio and exit pressure and turbine's non-dimensional speed.
  - Efficiency of the components at their working point and efficiency of the cycle.

For properties necessary during the calculation, City uses iterative procedures which give the required properties based on the composition of the fluid, temperature and pressure (when needed). This give the values within the 1% or better accuracy range.