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3. The gas properties

3.1. Various models of gas

The kinetic theory of gases makes it possible to define the pressure and temperature in relation to the statistical effect of the collision of molecules against solid walls and to kinetic energy of thermal agitation. Different models of gas are deduced from this theory. They are implemented in the *PNGD00* submodel that is linked with the following icon:

$$\begin{cases} F = \frac{T_a}{r_a} = -\frac{T_b}{r_b} \\ V = -r_b w_b = r_a w_a \end{cases}$$

Several customized submodels of *PNGD00* are available.

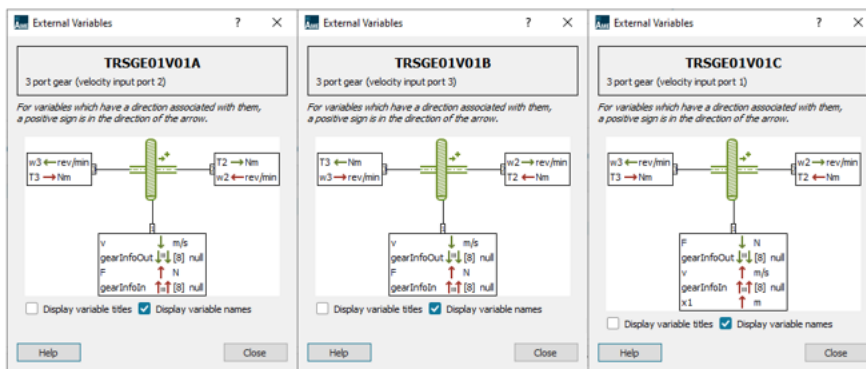


Fig. 3.1 *PNGD00* and its customized submodels

3.2. The gas type index parameter

All submodels from the **Pneumatic** library require a parameter called the **gas type index**, whose function is to reference a particular gas.

In the first tutorial example, the gas type index was equal to 1. This index is used to make the link between the properties of the gas and the submodels of the system which requires these properties to compute the enthalpy flow rates, the mass flow rates, the pressures or the temperatures. Display the parameter pop-up of submodel *PNCH022-1* (representing the first chamber) of the first tutorial example as shown in [Fig. 3.2](#).

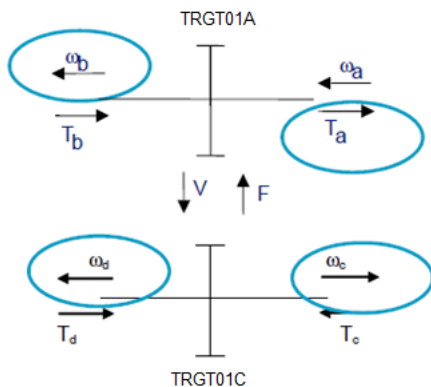


Fig. 3.2 Pneumatic chamber parameter pop-up

This submodel requires the gas type index, whose default value is 1. If you only have one gas in your system, you can leave the gas type index in *PNGD00* and in any other **Pneumatic** submodel at its default value.

The important rule is: **an icon associated with submodel *PNGD00* inserted on the sketch of a system refers to one and only one gas**. If your system has more than one gas, you must add the corresponding number of icons.

3.3. Defining the properties of the gas [1](#)

Pneumatic submodels may be supplied with the properties of the gas to compute the different variables exchanged at ports. Submodel *PNGD00* and its customized submodels are used to provide access to various properties fully defining a gas: the **equation of state**, the **constant-pressure specific heat**, the **absolute viscosity** and the **thermal conductivity**.

In generic submodel *PNGD00*, users can set their own properties through various data files.

$$\begin{cases} w_c = \frac{r_a}{r_c} w_a \\ T_a = \frac{r_a}{r_c} (T_c - T_d) + T_b \end{cases} \quad \begin{cases} w_b = w_a \\ w_d = -w_c \end{cases}$$

Fig. 3.3 Parameters of generic *PNGD00* [1](#)

In customized submodels of *PNGD00*, all properties are predefined. The user can only change the level of modeling.

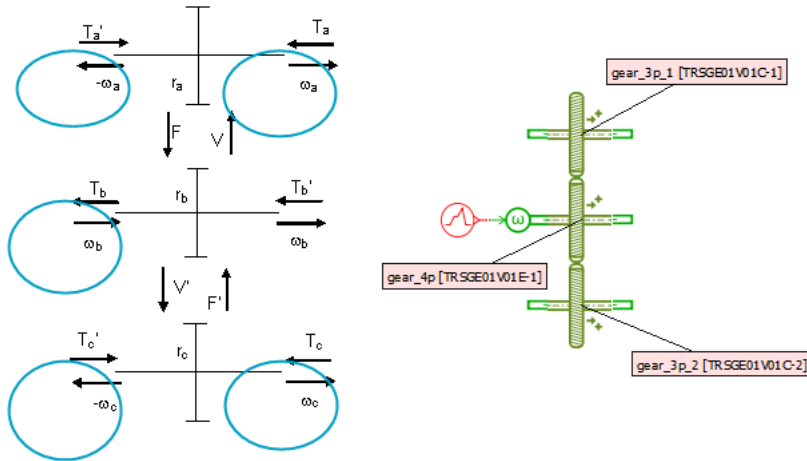


Fig. 3.4 Parameters of customized submodels of *PNGD00* [1](#)

There are three levels of modeling:

- **perfect gas**: the perfect equation of state is used. All other properties are constant.
- **semi-perfect gas**: the perfect equation of state is used. All other properties are temperature-dependent.
- **real gas**: a specific equation of state (among 4 predefined) is used. The absolute viscosity and the thermal conductivity are temperature-dependent. All other properties are temperature and pressure-dependent.

3.3.1. Perfect gas constant of a gas [1](#)

In the **Pneumatic** library, the perfect gas constant r of a gas referenced by an index is assumed to be constant. Therefore, there is no variation of the perfect gas constant when the temperature varies.

It is used in the perfect gas equation:

$$(3.1) \quad p \cdot V = m \cdot r \cdot T$$

The perfect gas constant is linked with the molar mass M of the gas through the perfect gas constant $R = 8.3145 \text{ J/mol/K}$:

$$(3.2) \quad r \cdot M = R$$

The perfect gas constant of the gas is expressed in J/kg/K .

3.3.2. Equation of state of a gas [1](#)

The equation of state is used to compute the density (ρ in kg/m^3) as a function of the pressure P and the temperature T .

3.3.2.1. Perfect gas or semi-perfect gas [1](#)

Perfect or semi-perfect gases use the perfect gas equation of state:

$$(3.3) \quad \rho = \frac{P}{r \cdot T}$$

3.3.2.2. Real gas [1](#)

Real gases use a specific equation of state from among four predefined:

- Van der Waals

$$(3.4) \quad \left(P + \frac{a}{V^2} \right) \cdot (V - b) - r \cdot T = 0$$

where the attractive term a and the covolume b are functions of the critical pressure, the critical temperature, and the perfect constant as written hereafter:

$$(3.5) \quad a = \frac{27 \cdot r^2 \cdot T_c^2}{64 \cdot P_c} \quad \text{and} \quad b = \frac{r \cdot T_c}{8 \cdot P_c}$$

- Redlich-Kwong

$$(3.6) \quad \left(P + \frac{a \cdot \alpha(T)}{V \cdot (V + b)} \right) \cdot (V - b) - r \cdot T = 0$$

where a and b coefficients are evaluated with the following relationships:

$$(3.7) \quad a = 0.42748024 \cdot \frac{r^2 \cdot T_c^{2.5}}{P_c} \quad \text{and} \quad b = 0.08664035 \cdot \frac{r \cdot T_c}{P_c}$$

the attractive term is temperature-dependent through the alpha-function:

$$(3.8) \quad \alpha(T) = \frac{1}{\sqrt{T}}$$

- Redlich-Kwong-Soave:

the equation of state is identical to the previous one proposed by Redlich-Kwong ([Eq.3.6](#)) but parameters and the alpha-function are different:

$$(3.9) \quad a = 0.42748024 \cdot \frac{r^2 \cdot T_c^2}{P_c} \quad \text{and} \quad b = 0.08664035 \cdot \frac{r \cdot T_c}{P_c}$$

$$(3.10) \quad \alpha(T) = \left[1 + m \cdot \left(1 - \sqrt{\frac{T}{T_c}} \right) \right]^2$$

with m calculated using a 2nd order polynomial function of the acentric factor:

$$(3.11) \quad m = 0.48 + 1.574 \cdot \omega - 0.176 \cdot \omega^2$$

ω is the Pitzer' s acentric factor, which is an intrinsic property of the gas considered, defined as follows:

$$(3.12) \quad \omega = -1 - \log_{10} \left(\frac{P_{\text{sat}}}{P_c} \right)_{T=0.7 \cdot T_c}$$

- Peng-Robinson

$$(3.13) \quad \left(P + \frac{a \cdot \alpha(T)}{V^2 + 2 \cdot b \cdot V - b^2} \right) \cdot (V - b) - r \cdot T = 0$$

where a and b coefficients are evaluated with the following relationships:

$$(3.14) \quad a = 0.457235583 \cdot \frac{r^2 \cdot T_c^2}{P_c} \quad \text{and} \quad b = 0.07779607 \cdot \frac{r \cdot T_c}{P_c}$$

The attractive term is temperature-dependent through the following alpha-function:

$$(3.15) \quad \alpha(T) = \left[1 + m \cdot \left(1 - \sqrt{\frac{T}{T_c}} \right) \right]^2$$

$$(3.16) \quad m = 0.37464 + 1.54226 \cdot \omega - 0.26992 \cdot \omega^2$$

This last model is the most accurate for processes occurring near the critical point.

Note

It is pointless to perform a simulation using the real gas submodel and the mixture submodel and/or selecting the polytropic model in pipe or volume submodels. Indeed, these computations will not take the real gas behavior into account.

3.3.3. Constant-pressure specific heat of a gas

The base formulation of the constant-pressure specific heat of a gas is its term that depends on the temperature. In the **Pneumatic** library this term comes from NASA literature (see [2] and [7]).

$$(3.17) \quad C_{p,NASA} = r \cdot \left(\frac{a_1}{T^2} + \frac{a_2}{T} + a_3 + a_4 \cdot T + a_5 \cdot T^2 + a_6 \cdot T^3 + a_7 \cdot T^4 \right)$$

The coefficients a_1 to a_7 are constant. They can be defined differently in various temperature ranges. For example, for air:

$$\begin{cases} w_a = -\frac{r_b}{r_a} w_b \\ w_c = -\frac{r_b}{r_c} w_b \end{cases}$$

Fig. 3.5 Example of definition for Cp for air

The specific heat of the gas is expressed in J/kg/K.

Note

A quadratic extrapolation is done when the current temperature falls outside the definition range.

3.3.3.1. Perfect gas

The constant-pressure specific heat is a constant.

$$(3.18) \quad C_p(P, T) = C_{p,0}$$

3.3.3.2. Semi perfect gas

The constant-pressure specific heat is equal to the NASA formulation.

$$(3.19) \quad C_p(P, T) = C_{p,NASA}(T)$$

3.3.3.3. Real gas

The constant-pressure specific heat is equal to the NASA formulation plus a residual term that depends on the equation of state.

$$(3.20) \quad C_p(P, T) = C_{p,NASA}(T) + C_{p,res}(P, T)$$

3.3.4. Thermal conductivity of a gas

The formulation of the thermal conductivity of a gas is a term that depends on the temperature. This term comes from NASA literature (see [2] and [7]).

$$(3.21) \quad \ln(\lambda(T)) = \ln(\lambda_{NASA}) = a_\lambda \cdot \ln(T) + \frac{b_\lambda}{T} + \frac{c_\lambda}{T^2} + d_\lambda$$

a_λ to d_λ coefficients are constant. They can be defined differently in various temperature ranges. For example, for air:

$$T_b = -\frac{r_b}{r_a}(T_a - T_a') - \frac{r_b}{r_c}(T_c - T_c') + T_b'$$

- the constant-volume specific heat is computed with the generalized Mayer law:

$$(3.23) \quad C_v = C_p - T \cdot \left(\frac{\partial P}{\partial T} \right)_v \cdot \left(\frac{\partial V}{\partial T} \right)_p$$

- the kinematic viscosity of the gas:

$$(3.24) \quad \nu = \frac{\mu}{\rho}$$

- the specific heat ratio of the gas:

$$(3.25) \quad \gamma = \frac{C_p}{C_v}$$

- the isentropic calorific factor of the gas:

$$(3.26) \quad \gamma_s = \frac{C_v}{C_p} \cdot \gamma_T$$

where γ_T is the isothermal calorific factor of a gas which is defined hereafter:

$$(3.27) \quad \gamma_T = -\frac{P}{v} \cdot \left(\frac{\partial v}{\partial P} \right)_T$$

where v is the specific volume [m³/kg].

These calorific factors are dependent on the gas model chosen or on the equation of state chosen to describe the gas behavior. For example, considering the perfect or semi-perfect (ideal) gas assumption, the isothermal calorific factor is equal to one, and so, the isentropic calorific factor is equal to the inverse of the specific heat ratio:

$$(3.28) \quad \gamma_s = \frac{1}{\gamma}$$

- the speed of sound:

$$(3.29) \quad c_s = \sqrt{\left(\frac{\partial P}{\partial \rho} \right)_S} = \sqrt{\gamma \cdot \left(\frac{\partial P}{\partial \rho} \right)_T}$$

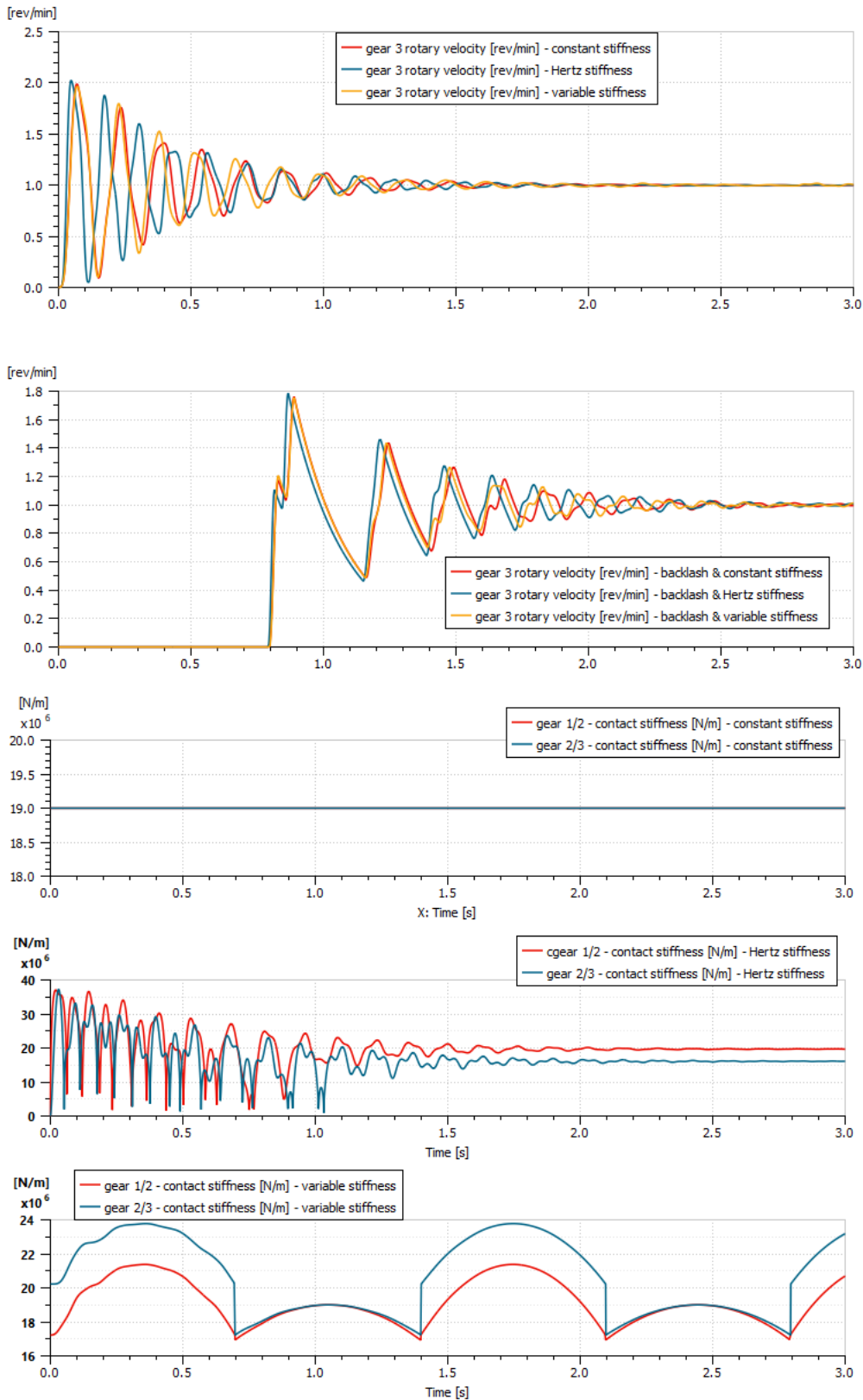
where S stands for entropy.

Considering a perfect or semi-perfect (ideal) gas behavior, the previous definition of the speed of sound becomes:

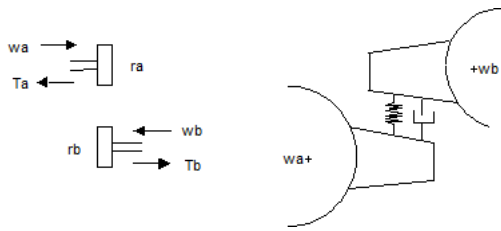
$$(3.30) \quad c_s = \sqrt{\gamma \cdot r \cdot T}$$

3.4. Setting/viewing gas properties in Simcenter Amesim [1](#)

A specific app is available at *PNGD00* level to change and view the gas properties. This app can be launched directly when double-clicking or right-clicking on the *PNGD00* icon or in its parameters view.



The app shows properties as a function of temperature for a given pressure. The level of modeling can be changed to quickly assess the variations of properties it generates.

Fig. 3.8 “gas_properties_app” [1](#)

As said above, the properties of a perfect gas are constant. Perfect gas constant and constant-pressure specific heat can be set through a pair of thermodynamics values.

$$F_{contact} = K_{contact} q_{relative} + D_{contact} w_{relative}$$

Fig. 3.9 Setting a user-defined “perfect” gas [1](#)

For predefined gas (customized submodels of *PNGD00*) it is possible to set the constant properties out of a given operating temperature and existing defined properties supposing a semi-perfect level of modeling.

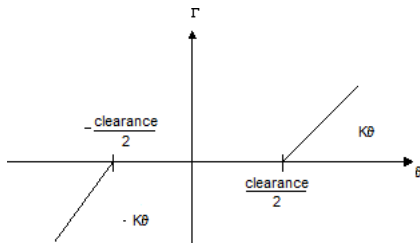
Fig. 3.10 Setting a predefined “perfect” gas [1](#)

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