Users' Guide for PC-TAS

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Contents

1 General

PC-TAS (Phase Change Thermo Acoustic Simulator) is a software for simulation of 1D acoustics, thermoacoustics and phase change thermoacoustics. This guide includes instructions for operation of PC-TAS and a full mathematical description of all the models and equations employed.

Resources including installation files, video tutorials, code samples and example files are available at https://wetlab.net.technion.ac.il/pc-tas/

1.1 Installation

PC-TAS can be installed as a MATLAB application, requiring MATLAB 2020b or newer versions. This can be done by executing the .mlappinstall file with MATLAB running.

PC-TAS can also be installed as a stand-alone desktop application on Windows 10 (tested and recommended), as well as on earlier versions of Windows, Linux and Mac (not tested). The stand-alone installation can be done by executing the .exe file, which will also install MATLAB runtime (a free software) automatically. Therefore, we recommend uninstalling all existing versions of MATLAB runtime before installation.

1.2 Interface

We built an user-friendly interface for the simulation of thermoacoustic systems. It consists of four tabs: Drag and drop, Tables, Graphs and Calculator.

1.2.1 Drag and drop

As shown in Fig. 1, this interface allows the users to drag a component from the new component list in the right top corner, and drop it in the system-building area to build a thermoacoustic system.

Guess & Targets in the left top corner lists all the values of guesses and targets.

In the area of system properties, all the global parameters (e.g., frequency, mean pressure, working fluid, dry or wet, etc.) and the values of pressure, volumetric velocity and temperature and the begnining of the model, can be set here.

The sand Box is used to investigate components separately, without insertion into the system. the component and its different properties can be reviewed, while system convergance is maintained.
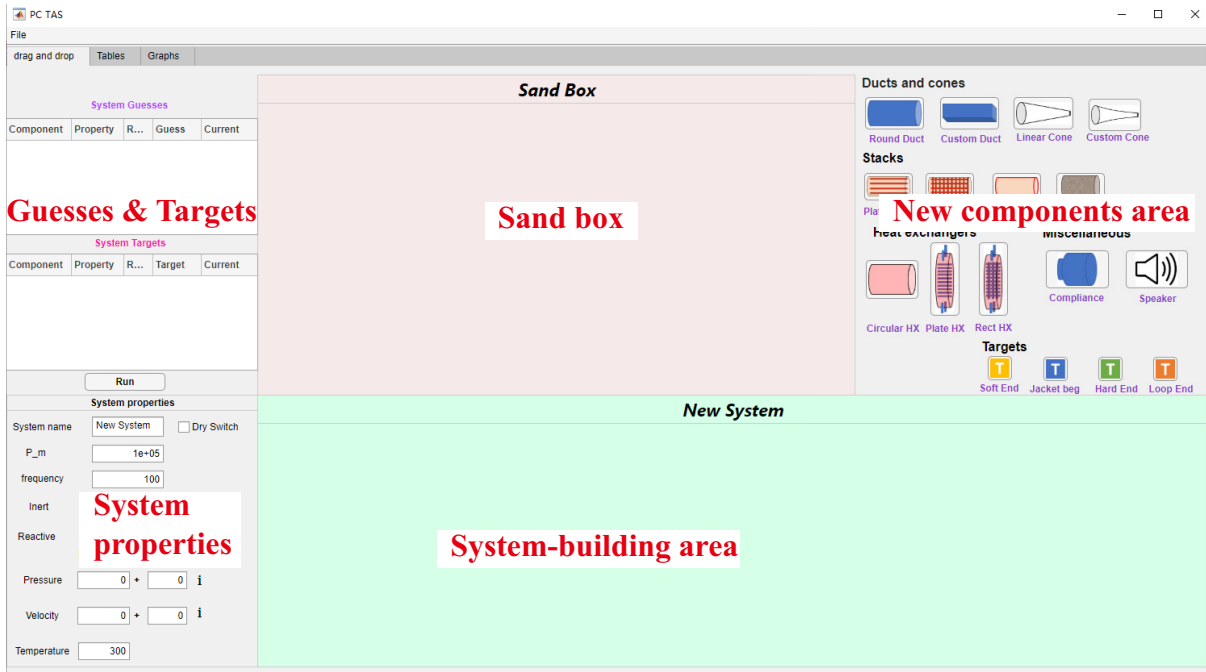
Figure 1: Interface of drag and drop.

A single component can be investigated and changed by right-clicking and then clicking "change properties".

1.2.2 Tables

The different system parameters, including both input parameters (length, diameter, area, etc.) and output parameters (pressure amplitude, volumetric velocity amplitude, temperature, etc.), are all listed in the "Tables" tab with a convenient interface, much like that in the software DELTAEC (Ward et al., 2008).

1.2.3 Graphs

After the system is run, the distributions of pressure, volumetric velocity, temperature, acoustic power, total power and mass flux are plotted and displayed here automatically.

1.2.4 Calculator

This interface allows the user to calculate and display the fluid properties of a chosen fluid at chosen conditions. The left side of the tab displays a table that collects the properties themselves. The right side displays a graph of up to two chosen properties, with a changing temperature and constant pressure.

1.3   Building a system

We provide various components that cover the requirement for building most thermoacoustic systems. A system can be built by the following simple steps:

1. Drag the first component of your system from the component list and drop it into the system-building area. You need to set the name and parameters of the component (listed as "Initial Parameters Defintion") when you drop it.

2. Repeat the first step to drag and drop all the components of your system one by one, until the full system is assembled.

3. Set the begin parameters in the left bottom corner.

4. Set guesses and targets in the left top corner. Note that the numbers of guesses and targets must be identical.

5. Set initial values to all the guesses. Note that it is very important to give relatively precise initial values, otherwise the algorithm may diverge.

6. Press "Run" button.

The users are suggested to start with the examples we offered.

1.4   Save and load a model

The model can be saved and loaded through the file menu at the top of the screen.

1.5   Data acquisition

After the run operation is done, the converged results and the general information of the model can be output into two .mat files, through click the "Export Data" in the "File" list. Table files and pictures of the graphs will be generated as well.

2 Math and algorithm

The mathematical model we used in this software can be summarised by Eqs.(1) to (3) in the article (Yang R and G.Z, 2022). The specific equations used in each component can be found in the following chapters.

A shooting method (the Hybrid Powel method (Powell, 1970)) is used to solve the guesses, i.e., the unknown parameters and initial conditions in the model. In order to do this, the targets whose amount must be identical to that of the guesses must be provided. Additionally, the shooting method requires initial values for all guesses. Values far away from the precise values will lead to the failure of the algorithm, i.e., the diverged results. In this case, the code will shoot one (or several) more time automatically by slightly changing the initial guess: all guess values are multiplied by random numbers in the range of 0.95-1.05. This improves the success rate to get converged results.

3   Physical segments

All the physical segments of the thermoacoustic systems are simulated by the corresponding code objects. In each object, the distributions of oscillating pressure, oscillating velocity and mean temperature are solved according to the correponding governing equations when the system is run. The acoustic power is calculated by $\dot{E}_2 = \frac{1}{2} \, \Re \left[p_1 \tilde{U}_1 \right]$. The total power in the system, representing the amount of energy transferred by the acoustic wave, is treated differently in different sections, as described in the description of each segment.

3.1   Duct

Ducts are the most basic element of an acoustic system. The sound wave propagates along the duct, attenuated by viscous, thermal and diffusive effects. In all available kinds of ducts, the governing equations are:

$$\frac{dp_1}{dx} = -\frac{i\omega \rho_m}{F_\nu A_{gas}} U_1 \tag{1}$$

$$\frac{dU_1}{dx} = -\frac{i\omega A_{\text{gas}}}{\rho_m a^2} \left[1 + (\gamma - 1)(1 - F_\alpha) + \gamma \frac{C_{\text{m}}}{1 - C_{\text{m}}} \frac{1 - F_D}{\eta_{\text{D}}} \right] p_1 \tag{2}$$

where

$$F_n = \begin{cases} 1 - (1 - i)\delta_n/2r_h, & \text{if } r_h/\delta_n > 15 \\ 1 - \frac{2J_1[(i-1)2r_h/\delta_n]}{J_0[(i-1)2r_h/\delta_n](i-1)2r_h/\delta_n} & \text{if } r_h/\delta_n < 12.5 \end{cases} \tag{3}$$

where $n = \alpha, \nu, D$. If $12.5 \leq r_h/\delta_n \leq 15$, the value of F_n will be interpolated accordingly.

Turbulence may occur in the duct. To specify the turbulence, we define the Peak Reynolds number in the oscillatory flow:

$$|Re_1| = \frac{4|U_1|r_h\rho_m}{A\mu}. \tag{4}$$

The criterion for turbulence is

$$\begin{cases} |Re_1|\frac{\delta_\nu}{2r_h} > 1000, & \text{if } r_h/\delta_\nu > 1 \\ |Re_1| > 2000 & \text{if } r_h/\delta_\nu < 1 \end{cases} \tag{5}$$

To account for the effects of turbulence, a correction factor m_ν is introduced (Swift, 2003):

$$m_\nu = \frac{\delta_\nu^2 |Re_1|}{24\pi r_h^2} \frac{f_m - (1 - 9\pi/32)|Re_1|f_m'}{\Re\left[i/\left(1 - f_\nu\right)\right]}. \tag{6}$$

The moody factor f_m and it's derivative $f_m' = \frac{df_m}{d|Re_1|}$ are calculated by solving the iterative equation (Chichester and Huber, 2008):

$$\frac{1}{\sqrt{f_m}} = 1.7385 - 2log_{10}\left(0.001 + \frac{18.574}{|Re_1|\sqrt{f_m}}\right). \tag{7}$$

The viscocity function F_ν is then modified by:

$$F_{\nu,tub} = \left[m_\nu \Re \left(\frac{1}{F_\nu} \right) + m_\nu^* \Im \left(\frac{1}{F_\nu} \right) \right]^{-1}, \tag{8}$$

where $\Im$ signifies an imaginary part of a complex number, and

$$m_\nu^* = \left(\frac{1 - \delta_\nu/2r_h}{1 - \delta_\nu/m_\nu 2r_h} \right)^2. \tag{9}$$

Due to the enhanced heat and mass transfer, the turbulence also amplifies losses due to thermal and diffusive relaxation in the duct. To account for this, the thermal and diffusive functions F_α and F_D are also modified by m_ν. This approximation has been used in DLETAEC for the thermal relaxation alone, and would benefit from theoretical or experimental justification.

3.1.1 RoundDuct

A duct with a circular cross section.

Initial Parameters Definition:

Length [m]: length of the duct.

Diameter [m]: diameter of the duct D.

Additional parameters:

Area [m^2]: cross-sectional area A_{gas} of the duct, linked to the diameter by $A = \pi D^2/4$

Rh [m]: hydraulic radius of the duct r_h, linked to the diameter by $r_h = D/4$

Jacket: If it is on, $\dot{H}_2 = \dot{E}_2$; if it is off, $\dot{H}_2$ is inherited from the preceding component.

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

3.1.2 CustDuct

A duct with an arbitrarily shaped cross section, specified by the hydraulic radius and the cross-sectional area, which are independent of each other.

Initial Parameters Definition:

Length [m]: length of the duct.

Area [m^2]: cross-sectional area A_{gas} of the duct.

Rh [m]: hydraulic radius r_h of the duct.

Additional parameters:

Jacket: whether or not the duct is water jacketed.

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

3.2 Cone

A cone is essentially a duct with a variable cross section. The governing equations are identical to the ones for a duct but with changing cross-sectional area.

3.2.1 LinearCone

A cone with a circular cross section whose diameter changes linearly along the axial direction.

Initial Parameters Definition:

Length [m]: Length.

D_1 [m]: Diameter at initial point in the cone.

D_2 [m]: Diameter at the final point in the cone.

Additional parameters:

rh_1 [m]: Hydraulic Radius at initial point in the cone. linked to the Diameter by $rh_1 = D_1/4$

rh_2 [m]: Hydraulic Radius at final point in the cone. linked to the Diameter by $rh_2 = D_2/4$

A_1 [m^2]: Area at initial point in the cone. linked to the Diameter by $A_1 = \pi D_1^2/4$

A_2 [m^2]: Area at final point in the cone. linked to the Diameter by $A_2 = \pi D_2^2/4$

Jacket: whether or not the cone is water jacketed

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

3.2.2 CustCone

Represents a custom Cone, with arbitrarily varying hydraulic radius and Area.

Initial Parameters Definition:

Length [m]: length of the cone.

Rh_1 [m]: Hydraulic Radius at initial point in the cone.

Rh_2 [m]: Hydraulic Radius at the final point in the cone.

A_1 [m^2]: Area at initial point in the cone.

A_2 [m^2]: Area at final point in the cone.

Additional parameters:

Mode A: The manner in which Area changes along the axial direction. The area will always change between A1 to A2. The mode could be one of the following: linear, exponent+ (e^X), exponent- (e^{-x}), square (x^2) and sqrt ($\sqrt{x}$)

Mode R: The manner in which hydraulic Radius changes along the axial direction. The radius will always change between Rh1 to Rh2.

Jacket: whether or not the cone is water jacketed

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

3.3   Heat Exchangers

Heat Exchangers allow the addition or removal of heat to and from the system. They also have a substantial effect on the acoustic wave itself, usually attenuating it due to their small pores. In all heat exchangers, the temperature is assumed constant and the governing equations are:

$$\frac{dp_1}{dx} = -\frac{i\omega\rho_m}{F_\nu A_{gas}} U_1 \tag{10}$$

$$\frac{dU_1}{dx} = -\frac{i\omega A_{\text{gas}}}{\rho_m a^2}\left[1 + \frac{(\gamma-1)\left(1-F_\alpha\right)}{1+\epsilon_s} + \gamma\frac{C_m}{1-C_m}\frac{1-F_D}{\eta_D}\right] p_1 \tag{11}$$

the heat transfer between the fluid and the solid is done through convection, and the convection coefficient is evaluated by

$$h = \frac{\alpha}{\min\left[\delta_\alpha, r_h\right]}. \tag{12}$$

Then the solid temperature of the heat exchanger can be calculated by Netwon's law of heating,

$$T_{solid} = T_m + \frac{\dot{Q}}{hA_{eff}}, \tag{13}$$

where $A_{eff} = \frac{A}{r_h}\min\left[L, 2\xi_1\right]$ is the effective area for heat transfer. $\xi_1 = \frac{U_1}{A\omega}$ is the acoustic displacement and L is the heat exchanger's length. We Note that we ignore the influence of phase change on heat exchange. The calculation of F_i and ϵ_s is different in every kind of heat exchanger, as detailed below. The total power in all heat exchangers is increased in a value equal to the heat input of the heat exchanger.

3.3.1   PlateHX

In a plate heat exchanger, the geometry is a parallel plate geometry, and the functions F and ϵ_s are calculated by

$$F_n = 1 - \frac{\tanh\left[(1+i)Y_0/\delta_n\right]}{(1+i)Y_0/\delta_n}, \tag{14}$$

$$\epsilon_s = \left(\frac{k\rho_m c_p}{k_s\rho_s c_s}\right)^{1/2}\frac{\tanh\left((1+i)Y_0/\delta_\alpha\right)}{\tanh\left((1+i)l_p/\delta_s\right)} \tag{15}$$

Where $\delta_s = \sqrt{2\alpha_s/\omega}$ is the thermal penetration depth of the solid and the subscripit s denotes a property of the solid.

Initial Parameters Definition:

Length [m]: length.

Diameter [m]: Diameter of the Heat exchanger.

Y0 [m]: Half the distance between the plates in the HX Y_0.

Porosity [-]: Ratio of the gas area and the total area ϕ.

Q [W]: The heat input into the heat exchanger $\dot{Q}$.

Additional parameters:

Solid: The Solid material of which the heat exchanger is made

Area [m^2]: Area A. linked to the Diameter by $A = \pi D^2 / 4$

Solid Area [m^2]: Area covered by the solid. Linked to the Area and Porosity by $A_{solid} = (1 - \phi)A$.

lp [m]: Half the plate thickness in the HX l_p. Upon creation, it is linked to the Porosity and Y_0 by $l_p = \frac{Y_0}{Y_0 + l_p}$. Afterwards it can be changed freely and it is not linked.

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

Solid Temperature [K]: Temperature of the solid material T_{solid}. This property is calculated when the system is run and is not defined by the user.

3.3.2 RectHX

In a Rectangular heat exchanger, the geometry is a Rectangular pore geometry, and the functions F and ϵ_s are calculated by

$$F_n = \frac{64}{\pi^4} \sum_{\substack{m,n \\ \text{odd}}} \frac{1}{m^2 n^2 \left[1 - i \frac{\pi^2 \delta_n^2}{8 Y_1^2 Y_2^2} (Y_2^2 m^2 + Y_1^2 n^2) \right]}, \tag{16}$$

$$\epsilon_s = \left(\frac{k \rho_m c_p}{k_s \rho_s c_s} \right)^{1/2} \frac{(1 - F_\alpha)(1 + i) Y_1 Y_2 / \delta_\alpha (Y_1 + Y_2)}{\tanh \left[(1 + i) \ell / \delta_s \right]} \tag{17}$$

Where $\delta_s = \sqrt{2\alpha_s / \omega}$ is the thermal penetration depth of the solid and the subscript s denotes a property of the solid.

Initial Parameters Definition:

Length [m]: Length.

Diameter [m]: Diameter D

Y1 [m]: Half the width of the pores Y_1.

Y2 [m]: Half the height of the pores Y_2.

Porosity [-]: Ratio of the gas area and the total area ϕ.

Q [W]: The heat input $\dot{Q}$ into the heat exchanger

Additional parameters:

Solid: The solid material of the HX.

Area [m^2]: Area of the HX A. linked to the Diameter by $A = \pi D^2 / 4$

Solid Area [m^2]: Area covered by the solid. Linked to the Area and porosity by $A_{solid} = (1 - \phi)A$.

lp [m]: Half the wall thickness l_p. Upon creation, it is linked to the Porosity, Y_1 and Y_2 by $l_p = \frac{Y_1 Y_2 (1/\phi - 1)}{Y_1 Y_2}$. Afterwards it can be changed freely and it is not linked.

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

Solid Temperature [K]: Temperature of the solid material. This property is calculated when the system is

run and is not defined by the user.

3.3.3 TubesHX

In this heat exchanger, the geometry is a round pore geometry, and the function F is calculated based on Eq.(3). the function ϵ_s is calculated based on:

$$\epsilon_s = \left(\frac{k\rho_m c_p}{k_s \rho_s c_s}\right)^{1/2} \frac{1}{\tanh\left((1+i)r_h/\delta_s\right)} \tag{18}$$

Where $\delta_s = \sqrt{2\alpha_s/\omega}$ is the thermal penetration depth of the solid and the subscript s denotes a property of the solid.

Initial Parameters Definition:

Length [m]: Length.

D [m]: Diameter of the pores in the heat exchanger

Area [m^2]: Area A.

Solid Area [m^2]: Area covered by the solid A_{solid}.

Q [W]: The heat input into the heat exchanger $\dot{Q}$.

Additional parameters:

Solid: The solid material of which the heat exchanger is made

Porosity [-]: Ratio of the gas area and the total area. linked to the Area and solid area by $\phi = \frac{A - A_{solid}}{A}$

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

Solid Temperature [K]: Temperature of the solid material. This property is calculated when the system is run and cannot be changed by the user.

3.4 Stacks, regenerators and thermal buffer tubes

In this section we present all the components with a temperature gradient in them. These elements include the different kinds of stacks, which are the hearts of most thermoacoustic systems, as well as thermal buffer tubes. For all these components except MeshSTK, the governing equations are:

$$\frac{dp_1}{dx} = -\frac{i\omega\rho_m}{F_\nu A_{gas}}U_1 \tag{19}$$

$$\begin{aligned}
\frac{dU_1}{dx} = &-\frac{i\omega A_{\text{gas}}}{\rho_m a^2}\left[1 + \frac{(\gamma - 1)(1 - F_\alpha)}{1 + \epsilon_s} + \gamma\frac{C_{\text{m}}}{1 - C_{\text{m}}}\frac{1 - F_D}{\eta_{\text{D}}}\right]p_1 \\
&+ \left[\frac{F_\nu - F_\alpha}{(1 - Pr)(1 + \epsilon_s)F_\nu}\beta + \frac{\frac{\eta_\nu}{\eta_{\text{D}}}(1 - F_D) - (1 - F_\nu)}{F_\nu(1 - Sc)}\frac{C_{\text{m}}}{1 - C_{\text{m}}}\frac{l_{\text{h}}}{R_{\text{g}}T_{\text{m}}^2}\right]\frac{dT_m}{dx}U_1
\end{aligned} \tag{20}$$

$$\frac{dT_m}{dx} = \frac{\dot{H}_2 - \frac{1}{2}\Re\left[p_1\widetilde{U}_1\left(1 - \frac{\tilde{F}_\nu - F_\alpha}{(1+Pr)(1+\epsilon_s)\widetilde{F}_\nu}\right)\right] - \dot{m}l_h}{\frac{\rho_m c_p |U_1|^2}{2A_{\text{gas}}\omega(1-Pr)|F_\nu|^2}\Im\left[\frac{(\widetilde{F}_\nu - F_\alpha)[1+\epsilon_s(1-F_\nu)/(1-F_\alpha)]}{(1+Pr)(1+\epsilon_s)} - \widetilde{F}_\nu\right] - (A_{\text{gas}}k + A_s k_s)} \tag{21}$$

where

$$
\begin{aligned}
\dot{m} =\; & \frac{1}{1-C_m}\frac{C_m}{2R_g T_m}\Re\left[p_1\widetilde{U}_1\frac{F_D - \widetilde{F}_v}{(1+Sc)\widetilde{F}_v}\right] \\
& - \frac{1}{1-C_m}\frac{|U_1|^2}{2A_{\text{gas}}\omega\,|F_v|^2}\frac{p_m C_m l_h}{R_g^2 T_m^3}\frac{1}{1-Sc^2}\Im\left[\widetilde{F}_v(1+Sc) + \frac{\eta_v}{\eta_D}\left(F_D - \widetilde{F}_\nu\right)\right]\frac{dT_m}{dx} \\
& - \frac{p_m A_{\text{gas}} D}{1-C_m}\frac{C_m l_h}{R_g^2 T_m^3}\frac{dT_m}{dx}
\end{aligned}
\tag{22}
$$

And the difference is in the calculation method for F_i and ϵ_s. The total power remains constant in all stacks.

3.4.1 PlateSTK

A stack or regenerator with parallel-plates geometry. F and ϵ are calculated based on Eq. (14) and Eq. (15) repectively.

Initial Parameters Definition:

Length [m]: Length.

Diameter [m]: Diameter D.

Y0 [m]: Half the plate spacing Y_0.

Porosity [-]: Ratio of the gas area and the total area ϕ.

Additional parameters:

Solid: The solid material.

Area [m^2]: Area A. linked to the diameter by $A = \pi D^2/4$

Solid Area [m^2]: Area covered by the solid. Linked to the Area and Porosity by $A_{solid} = (1-\phi)A$.

lp [m]: Half the plate thickness in the HX l_p. Upon creation, it islinked to the Porosity and Y_0 by $l_p = \frac{Y_0}{Y_0+l_p}$ Afterwards it can be changed freely and it is not linked.

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

3.4.2 RectSTK

A Stack or regenerator with Rectangular pores geometry. F and ϵ_s are calculated based on Eq. (16) and Eq. (17) repectively.

Initial Parameters Definition:

Length [m]: Length.

Diameter [m]: Diameter D.

Y1 [m]: Half the Width of the pores Y_1.

Y2 [m]: Half the Height of the pores Y_2.

Porosity [-]: Ratio of the gas area and the total area ϕ.

Additional parameters:

Solid: The Solid material of which the stack is made

Area [m^2]: Area A. linked to the Diameter by $A = \pi D^2/4$

Solid Area [m^2]: Area covered by the solid. Linked to the Area and Porosity by $A_{solid} = (1 - \phi)A$.

lp [m]: Half the wall thickness l_p. Upon creation it is linked to the Porosity, Y_1 and Y_2 by $l_p = \frac{Y_1 Y_2 (1/\phi - 1)}{Y_1 Y_2}$.
Afterwards it can be changed freely and it is not linked.

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

3.4.3 CircSTK

A Stack or regenerator with circular pores geometry. and the function F is calculated based on Eq.(3). the function ϵ_s is calculated based on:

$$\epsilon_s = \left(\frac{k\rho_m c_p}{k_s \rho_s c_s} \right)^{1/2} \frac{(1 - F_\alpha)(1 + i)D/(4\delta_\alpha)}{\tanh\left((1 + i)r_h/\delta_s\right)} \tag{23}$$

Where $\delta_s = \sqrt{2\alpha_s/\omega}$ is the thermal penetration depth of the solid and the subscript s denotes a property of the solid.

Initial Parameters Definition:

Length [m]: Length.

Diameter [m]: Diameter D of the pores in the stack.

Area [m^2]: Area A. Porosity [-]: Ratio of the gas area and the total area ϕ.

lp [m]: Half the wall thickness

Additional parameters:

Solid: The Solid material of which the stack is made

Solid Area [m^2]: Area covered by the solid A_{solid}. It is linked to the Area and Porosity by $A_{solid} = (1 - \phi)A$.

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

3.4.4 TBT

A thermal buffer tube- a tube with thermo-acoustic conversion occuring on the boundary, leading to a temperature gradient on it. F_n is calculated according to Eq. (3). ϵ_s is expressed as

$$\epsilon_s = \left(\frac{k\rho_m c_p}{k_s \rho_s c_s} \right)^{1/2} \frac{1}{\tanh\left[(1 + i)\ell/\delta_s\right]}, \tag{24}$$

where ℓ is the wall thickness.

Initial Parameters Definition:

Length [m]: Length.

Diameter [m]: Diameter D.

lp [m]: Wall thickness ℓ.

Additional parameters:

Solid: The solid material

Area [m^2]: Area A, linked to the Diameter by $A = \pi D^2/4$

Rh [m]: Hydraulic radius r_h. linked to the Diameter by $r_h = D/4$

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

3.4.5 MeshSTK (dry only)

It represents a regenerator made of stacked mesh screens. Due to the absence of a model for such a component in a phase change thermoacoustic system, it can only be used in the dry (classical) mode. the governing equations are:

$$\frac{dp_1}{dx} = -i\frac{\omega\rho_m}{A_{gas}}\left[1 + \frac{(1-\phi)^2}{2(2\phi-1)}\right]U_1 - \frac{\mu}{r_h^2 A_{gas}}\left(\frac{c_1(\phi)}{8} + \frac{c_2(\phi)N_{R,1}}{3\pi}\right)U_1 \tag{25}$$

$$\frac{dU_1}{dx} = -\frac{i\omega\gamma A_{gas}}{\rho_m a^2}p_1 + \beta\frac{dT_m}{dx}U_1 +$$
$$i\omega\beta\left[\frac{A_{gas}T_m\beta}{\rho_m c_p}\frac{\epsilon_s + \left(g_c + e^{2i\theta_p}g_v\right)\epsilon_h}{1+\epsilon_s+\left(g_c+e^{2i\theta_T}g_v\right)\epsilon_h}p_1 - \frac{1}{i\omega}\frac{dT_m}{dx}\frac{\epsilon_s + (g_c - g_v)\epsilon_h}{1+\epsilon_s+\left(g_c+e^{2i\theta_T}g_v\right)\epsilon_h}U_1\right] \tag{26}$$

$$\frac{dT_m}{dx} = \left\{\mathrm{Re}\left[\left(T_m\beta\frac{\epsilon_s+\epsilon_h\left(g_c+e^{2i\theta_p}g_v\right)}{1+\epsilon_s+\epsilon_h\left(g_c+e^{2i\theta_T}g_v\right)}+1-T_m\beta\right)p_1\widetilde{\frac{U_1}{A_{gas}}}\right] - \frac{2\dot{H}_{2,k}}{\phi A}\right\}$$
$$\Big/\left\{\frac{\rho_m c_p}{\omega}\mathrm{Im}\left[\frac{\epsilon_s+\epsilon_h(g_c-g_v)}{1+\epsilon_s+\epsilon_h\left(g_c+e^{2i\theta_T}g_v\right)}\right]\left(\frac{|U_1|}{A_{gas}}\right)^2 + 2\left[k_{s,\mathrm{eff}}\frac{1-\phi}{\phi}+k\right]\right\} \tag{27}$$

where

$$c_1(\phi) = 1268 - 3545\phi + 2544\phi^2 \tag{28a}$$

$$c_2(\phi) = -2.82 + 10.7\phi - 8.6\phi^2 \tag{28b}$$

$$b(\phi) = 3.81 - 11.29\phi + 9.47\phi^2 \tag{28c}$$

$$N_{R,1} = 4\,|U_1|\,r_h\rho_m/\mu A_{gas} \tag{28d}$$

$$\theta_p = \text{phase}\,(U_1) - \text{phase}\,(p_1) \tag{28e}$$

$$\theta_T = \text{phase}\,(U_1) - \text{phase}\,(\langle T\rangle_{u,1}) \tag{28f}$$

$$g_c = \frac{2}{\pi}\int_0^{\pi/2} \frac{dz}{1 + N_{R,1}^{3/5}\cos^{3/5}(z)} \tag{28g}$$

$$g_v = -\frac{2}{\pi}\int_0^{\pi/2} \frac{\cos(2z)dz}{1 + N_{R,1}^{3/5}\cos^{3/5}(z)} \tag{28h}$$

Initial Parameters Definition:

Length [m]: Length.

Area [m^2]: Area A.

Solid Area [m^2]: Area covered by the solid.

Rh [m]: hydraulic radius r_h.

Solid: The solid material of which the mesh is made

k [-]: A factor governing the contribution of thermal conduction in the regenerator. A value of 0.1-0.3 is recommended.

Additional parameters:

Solid: The Solid material of which the stack is made

Nsolpoints: The number of solution points in the component. if no number is selected, the program will select the number by itself.

3.5   Loudspeakers

In thermoacoustic systems, the acoustic-electric transducers are often used to as a sound source or converted the generated acoustic power into electricity. In our code, we employ a lumped model for describing the electromagnetic transducers (e.g., linear alternator or loudspeaker, etc.) connected with the duct in series

(Swift, 2003):

$$p_{1,out} = p_{1,in} - \frac{BlI_1}{A_m} - \frac{R_m + i\left(\omega M - K/\omega\right)}{A_m^2} U_1^*, \tag{29}$$

$$U_1^* = U_{1,in} - \frac{\omega}{\rho_m a^2}\left(\gamma - 1\right)\frac{\delta_\alpha}{2} A_m p_{1,in}, \tag{30}$$

$$U_{1,out} = U_{1,in} - \frac{\omega}{\rho_m a^2}\left(\gamma - 1\right)\frac{\delta_\alpha}{2} A_m \left(p_{1,in} + p_{1,out}\right), \tag{31}$$

$$I_1 = \frac{V_1 + BlU_1^*/A_m}{R_e + i\omega L}, \tag{32}$$

where Bl is the transduction coefficient, I_1 is the oscillating current, A_m is the cross-sectional area of moving part of the transducer, V_1 is the oscillating voltage, R_m is the mechanical resistance of the loudspeaker, M is the mass of the spring-coil system and K is the spring constant. The electric power consumption of the loudspeaker is calculated by:

$$\dot{E}_e = 0.5\Re(V_1 I_1) \tag{33}$$

The total power in the loudspeaker either equals the acoustic power (in jacketed mode) or else it is increased by the electric power consumption.

Initial Parameters Definition:

Area [m^2]: Area of moving part A_m.

R_e [Ω] : Electric resistance R_e of the coil.

L [H]: Electric inductance L of the coil.

Bl [N/A]: Trnasduction coefficient Bl. Equals to the force exerted by the coil divided by the current in it.

M [kg]: Moving mass M.

K [N/m]: Mechanical stiffness K.

R_m [Ns/m]: Mechanical resistance R_m.

V [V]: Complex electric voltage V_1.

Additional parameters:

Jacket: Whether or not the compliance is water jacketed.

Electric Consumption [W]: Electric consumption of the loudspeakers. This property is calculated when the system is run and cannot be changed by the user.

3.6   Compliance

Represents a volumetric bulb serving as an acoustic compliance. The compliance is governed by the equations:

$$U_{1,\,out} = U_{1,\,in} - i\frac{\omega p_1}{\rho_m a^2}\left[V - i\frac{\gamma - 1}{1 + \epsilon_s}S\frac{\delta_\kappa}{2}\right] \tag{34}$$

where

$$\epsilon_s = \left(\frac{k\rho_m c_p}{k_s \rho_s c_s}\right)^{1/2}. \tag{35}$$

The values of p_1 and T_m remain constant in this component. The total power either equals the acoustic power, if the compliance is water jacketed, or remains constant otherwise.

Initial Parameters Definition:

Area [m^2]: Surface area S of the compliance.

Volume [m^3]: Volume V of the compliance.

Additional parameters:

Jacket: Whether or not the compliance is water jacketed.

3.7 Liquid Piston

Represents a liquid column inside the system, serving as a liquid piston. The water piston is governed by the equation (derived from Xu et al. (2020)) :

$$p_{1,out} = p_{1,in} - \frac{1}{A^2}\left(R_m + i\left(\omega\rho A L_{total} - 2\rho A g/\omega\right)\right)U_1 \tag{36}$$

where $R_m = \pi^{1.5}DL\sqrt{\rho\mu f} + 0.02625\pi\rho f|U_1|D^2/A$, and $D = \sqrt{4A/\pi}$ The values of U_1 and T_m remain constant in this component. The total power either equals the acoustic power, if the piston is water jacketed, or remains constant otherwise.

Initial Parameters Definition:

Length [m]: Components length, only used for plotting.

Density [kg/m^3]: Density ρ of the liquid.

d.Viscosity [$Pa\ s$]: Dynamic Viscosity μ of the fluid.

Area [m^2]: Area A of the piston.

L total [m]: Total length L_{total} of the liquid column.

Additional parameters:

Jacket: Whether or not the liquid piston is water jacketed.

Nsolpoints: The number of solution points in the component. Equals to 2 for this component.

3.8 Minor Loss

Represents minor loss effects due to bends, expansions, and other flow effects. The minor loss is governed by the equation:

$$P_{1,\ out} = P_{1,\ in} - K\frac{4\rho_m|U_1|}{3\pi A^2}U_1 \tag{37}$$

The values of U_1 and T_m remain constant in this component. The total power either equals the acoustic power, if the Minor Loss is water jacketed, or remains constant otherwise.

Initial Parameters Definition:

Area $[m^2]$: The area A on which the minor loss coefficient is based.

K [-]: Minor loss coefficient K.

Additional parameters:

Jacket: Whether or not the minor loss is water jacketed.

3.9   Transfer Matrix

Describes an impedance relation between the pressure and velocity before and after. The transfer matrix is governed by the equation:

$$\begin{pmatrix} P_{1,\text{ out}} \\ U_{1,\text{ out}} \end{pmatrix} = \begin{pmatrix} P_{1,\text{ in}} \\ U_{1,\text{ in}} \end{pmatrix} + \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} P_{1,\text{ in}} \\ U_{1,\text{ in}} \end{pmatrix} \tag{38}$$

The value of T_m remains constant in this component. The total power either equals the acoustic power, if the Transfer Matrix is water jacketed, or remains constant otherwise.

Initial Parameters Definition:

m_{11} [-]: Relates changes in the pressure to the pressure before the Transfer Matrix

m_{12} $[Pa * s/m^3]$: Relates changes in the pressure to the velocity before the Transfer Matrix

m_{21} $[m^3/Pa * s]$: Relates changes in the velocity to the pressure before the Transfer Matrix

m_{22} [-]: Relates changes in the velocity to the velocity before the Transfer Matrix

Additional parameters:

Jacket: Whether or not the transfer matrix is water jacketed.

4   Targets

Target components are used to add targets for the shooting algorithm, that are not the regular system parameters. each Target has a property "Target Value" that can be added to the system's target list

4.1   Jacket Target

A Jacket Target can be used at the transition point between an insulated and jacketed segment. It targets the difference between the acoustic and total power in a system:

$$TV = \dot{E} - \dot{H} \longrightarrow 0 \tag{39}$$

4.2   HardEnd

A HardEnd is used at boundary of a solid end (the closed end of a resonator, for instance), targeting the value of velocity, or the inverse of impedance $1/|Z|$, to be zero:

$$TV = \frac{1}{|Z|} = \frac{|U_1|}{|p_1|} \frac{\rho_m a}{A_{gas}} \longrightarrow 0 \tag{40}$$

4.3   SoftEnd

A SoftEnd is used at an open end or at the boundary of a large acoustic compliane, where the pressure amplitude or $|Z|$ is considered zero.

$$TV = |Z| = \frac{|p_1|}{|U_1|} \frac{A_{gas}}{\rho_m a} \longrightarrow 0 \tag{41}$$

4.4   LoopEnd

A LoopEnd Target is used to target a periodicity condition in looped systems. If the system is completely periodic (a full loop), the real and imaginary parts should be targeted to be zero, and the target function will be:

$$TV = (T, p_1, U_1) - (T_0, p_0, U_0) \tag{42}$$

where T_0, p_0, and U_0 are the mean Temperature at the begining of the system. if the system is periodic only in amplitude, the phase and amplitude can be targeted, and the target value will be.

$$TV = \left(\frac{p_1}{p_0}, \frac{U_1}{U_0} \frac{T_1}{T_0} \right) \tag{43}$$

the absolute value of the oscillating properties can be targeted to be 1, and the phase difference can be targeted at the relevant value.

5 Gases and solids

5.1 Gases

The following fluids are available as the working fluid: <u>Inert gases:</u> air, nitrogen, argon, helium, xenon, hydrogen, carbon dyoxide. <u>Reactive gases:</u> water, methanol, ethanol, isopropanol, ammonia, cyclopropane, propylene, propane, N_2O, acetone, butane, isobutane, dimethyl-ether, R218, ethane, R134a, R32.

The calculations for viscosity, diffusion coefficient and thermal conductivity are based on the kinetic theory of gases, as presented by Reid et al. (1987) A correction factor for highly polar substnces, as well as Hydrogen, was fitted for based on data from eThermo research team (2009). The values of latent heat and boiling temperature were fitted from data in eThermo research team (2009). The specific heat of cyclopropane, propane and $N_2$0 were fitted from eThermo research team (2009), while that of the other species from Reid et al. (1987). Lennard Jones potential parameters ($\epsilon/k_b, \sigma$) of dimethyl-ether were taken from Wang et al. (2011), of R134a from Wilhelm and Vogel (1996), of R32 and R218 from Chichester and Huber (2008), and the rest from Reid et al. (1987).

All of the formulas are valid in the temperature range where the ideal gas assumption is valid. ($P_m <<$ $P_c, T_m >> 0$) the software issues a warning at certain temperature ranges and pressure ranges, but it is the user's responsibility to make sure that the working range is appropriate. We usually use the properties within the range of $P_m < 20$ bar and 100 K$< T < T_b$, in which we believe that the data is reliable.

5.2 Mixture properties calculation

All properties of the mixture are calculated for a mixture of two gases, A and B. subscripts $()_A$ and $()_B$ represent properties of one of the gases only.

5.2.1 mass fraction

At all times, the mixture is assumed to be in equilibrium with a liquid layer of the reactive component. therefore, the mass fraction of the reactive component can be calculated by the Clausius Clapeyron relation.

$$C_m = \exp\left[-\frac{l_h}{R_g}\left(\frac{1}{T_m} - \frac{1}{T_b}\right)\right],$$
(44)

where l_h is the molar latent heat of the reactive component, T_b is the boiling temperature of the reactive component, and R_g is the universal gas constant. The boiling temperature and latent heat were fitted based on data from eThermo research team (2009).

5.2.2 Density

The density is calculated based on the ideal gas equation:

$$\rho = \frac{p}{TR_g/M_{mix}} \tag{45}$$

where $M_{mix} = C_m M_{reactive} + (1 - C_m)M_{inert}$ is the mixture molar mass.

5.2.3 Diffusion coefficient

The diffusion coefficient is calculated by

$$D_{AB} = 0.0018583\sqrt{T^3 \left(\frac{1}{M_A} + \frac{1}{M_B}\right)} \frac{1}{p\sigma_{AB}^2 \Omega_D(T^*)} \tag{46}$$

T^* is expressed as:

$$T^* = \frac{T}{\varepsilon_{AB}/k} \tag{47}$$

The parameters σ_{AB} and ϵ_{AB} are Lennard-Jones parameters and are calculated using known values σ_A, σ_B and ϵ_A, ϵ_B which are tabulated and the following equations (k is the Boltzmann coefficient)

For the mixture with non-polar components, the collisional integral π_D can be approximated using the following fit

$$\Omega_D = \frac{1.06036}{(T^*)^{0.15610}} + \frac{0.19300}{\exp\left(0.47635T^*\right)} + \frac{1.03587}{\exp\left(1.52996T^*\right)} + \frac{1.76474}{\exp\left(3.89411T^*\right)} \tag{48}$$

and

$$\sigma_{AB} = \frac{1}{2}\left(\sigma_A + \sigma_B\right) \tag{49}$$

$$\varepsilon_{AB} = \sqrt{\varepsilon_A \varepsilon_B} \tag{50}$$

If one or two components of the mixture are polar, a different collision integral relation is then necessary, and new Lennard-Jones parameters ϵ and σ are calculated. The new collision integral is then

$$\Omega_D(polar) = \Omega_D(nonpolar) + \frac{0.19\delta_{AB}^2}{T^*} \tag{51}$$

where

$$\delta = \frac{1.94 \cdot 10^3 \mu_p^2}{V_b T_b} \tag{52}$$

where μ_p is the dipole moment, V_b is the liquid molar volume at the normal boiling point and T_b is the normal boiling point. The Lennard-Jones parameters for each gas are calculated using the following relations

$$\varepsilon/k = 1.18\left(1 + 1.3\delta^2\right)T_b \tag{53}$$

$$\sigma = \left(\frac{1.585 V_b}{1 + 1.3\delta^2} \right)^{1/3} \tag{54}$$

And using the following means

$$\delta_{AB} = (\delta_A \delta_B)^{1/2} \tag{55a}$$

$$\varepsilon_{AB} = (\varepsilon_a \varepsilon_b)^{1/2} \tag{55b}$$

$$\sigma_{AB} = (\sigma_A \sigma_B)^{1/2} \tag{55c}$$

The liquid molar volume at the normal boiling point is calculated using

$$V_b = 0.285 V_c^{1.048}. \tag{56}$$

5.2.4 Viscosity

For a binary mixture of gases, the viscocity is calculated by:

$$\eta = 40.785 \frac{F_{cm}(M_m T)^{1/2}}{V_{cm}^{2/3} \Omega_v} \tag{57}$$

Ω_V is the collision integral used for viscosity and thermal conductivity coefficients, and is approximated by

$$\Omega_v = \frac{1.16145}{(T_m^*)^{0.14874}} + \frac{0.52487}{\exp(0.7732 T_m^*)} + \frac{2.16178}{\exp(2.43787 T_m^*)} \tag{58}$$

The term F_m is computed as follows

$$F_m = 1 - 0.275\omega_m + 0.059035\mu_{rm}^4 + \kappa_m \tag{59}$$

where

$$\mu_{rm} = \frac{131.3\mu_m}{(V_{cm} T_{cm})^{1/2}} \tag{60a}$$

$$V_{cm} = (\sigma_m/0.809)^3 \tag{60b}$$

$$T_{cm} = 1.2593(\varepsilon_m/k) \tag{60c}$$

κ is a special correction for highly polar substances that was tabluated by Reid et al. (1987). For alcohols it can be calculated by:

$$\kappa = 0.0682 + 4.704 \cdot \frac{\text{nuber of OH groups}}{\text{molecular weight}} \tag{61}$$

and for other polar substances that were not tabluated it was fitted for based on data from eThermo research team (2009). The parameters are calculated as follows:

$$T_m^* = \frac{T}{\varepsilon_m/k} \tag{62a}$$

$$\varepsilon_m/k = \frac{(\varepsilon_A/k)\,C_A^2\sigma_A^3 + (\varepsilon_B/k)\,C_B^2\sigma_B^3 + 2C_A C_B\,(\varepsilon_{AB}/k)\,\sigma_{AB}^3}{\sigma_m^3} \tag{62b}$$

$$M_m = \left[\frac{(\varepsilon_A/k)\,C_A^2\sigma_A^2 M_A^{1/2} + (\varepsilon_B/k)\,C_B^2\sigma_B^2 M_B^{1/2} + 2C_A C_B\,(\varepsilon_{AB}/k)\,\sigma_{AB}^2 M_{AB}^{1/2}}{(\varepsilon_m/k)\,\sigma_m^2}\right]^2 \tag{62c}$$

$$\sigma_m^3 = C_A^2\sigma_A^3 + C_B^2\sigma_B^3 + 2C_A C_B\sigma_{AB}^3 \tag{62d}$$

$$\omega_m = \frac{\omega_A C_A^2\sigma_A^3 + \omega_B C_B^2\sigma_B^3 + 2C_A C_B\omega_{AB}\sigma_{AB}^3}{\sigma_m^3} \tag{62e}$$

$$\mu_m^4 = \sigma_m^3\,(\varepsilon_m/k)\left[\frac{C_A^2\mu_A^4}{\sigma_A^3\,(\varepsilon_A/k)} + \frac{C_B^2\mu_B^4}{\sigma_B^3\,(\varepsilon_B/k)} + \frac{2C_A C_B\mu_A^2\mu_B^2}{\sigma_{AB}^3\,(\varepsilon_{AB}/k)}\right] \tag{62f}$$

$$\kappa_m = C_A^2\kappa_A + C_B^2\kappa_B + 2C_A C_B\kappa_{AB} \tag{62g}$$

σ and ε are calculated based on:

$$\sigma = 0.809 * V_c^{1/3} \tag{63a}$$

$$\varepsilon/k = \frac{T_c}{1.2593} \tag{63b}$$

And the combining rules are

$$\sigma_{AB} = (\sigma_A\sigma_B)^{1/2} \tag{64a}$$

$$\varepsilon_{AB}/k = \left(\frac{\varepsilon_A}{k}\frac{\varepsilon_B}{k}\right)^{1/2} \tag{64b}$$

$$\omega_{AB} = \frac{\omega_A + \omega_B}{2} \tag{64c}$$

$$\kappa_{AB} = (\kappa_A\kappa_B)^{1/2} \tag{64d}$$

$$M_{AB} = \frac{2M_A M_B}{M_A + M_B} \tag{64e}$$

5.2.5 Thermal conductivity

The thermal conductivity coefficient for a mixture of gases is calculated using the known viscosity value η_m obtained previously using the following equation

$$\lambda_m = 3.75\frac{\eta_m R_g\Psi}{M_m'} \tag{65}$$

R is the universal gas constant. The parameter Ψ is calculated using the following equation

$$\Psi = 1 + \alpha_m\left\{\frac{0.215 + 0.28288\alpha_m - 1.061\beta_m + 0.26665Z_m}{0.6366 + \beta_m Z_m + 1.061\alpha_m\beta_m}\right\} \tag{66}$$

using the following parameters

$$\alpha_m = \frac{c_{vm}}{R_g} - \frac{3}{2} \tag{67a}$$

$$\beta_m = 0.7862 - 0.7109\omega_m + 1.316\omega_m^2 \tag{67b}$$

$$Z_m = 2 + 10.5T_{rm}^2 \tag{67c}$$

Where C_{vm} is the mixture molar heat capacity, and . The value of β_m is obtained for non-polar gases using equation 67b, and for polar gases using tabulated values from Chung et al. (1984). If the compound is polar, and no known value of β is found, a default value of $\beta = 0.758$ is used.

5.2.6 Heat capacity

as stated earlier, c_{vm} is the constant heat capacity at constant volume [J/(mol K)] and is combined using the following rule

$$c_{vm} = c_{vA}C_A + c_{vB}C_B \tag{68}$$

c_v for monoatomic gases equals $1.5R_g$. With other gases we use a polynomial function of T

$$c_p/R = a_0 + a_1 10^{-3}T + a_2 10^{-5}T^2 + a_3 10^{-s}T^3 + a_4 10^{-11}T^4 \tag{69}$$

the values of a_0 to a_4 are either from Reid et al. (1987) or else fitted for from data by eThermo research team (2009). c_v and c_p : are linked by:

$$c_v = c_p - R_g \tag{70}$$

and the specific heat ratio is defined as $\gamma = c_p/c_v$.

5.2.7 Speed of sound

The speed of sound can be calculated by:

$$a = \sqrt{\gamma p_m/\rho} \tag{71}$$

5.3 Solids

The following solids are available in our code: ideal solid, copper, nickel, stainless steel, molybdenum, tungsten, mylar, kapton, celcor, ceramic.

Data of ceramic are from (Matweb, 2021 (accessed May 1, 2021), all the other data are obtained from Ward et al. (2008). As the valid temperature range there was not provided, the specific validity ranges of these expressions are not clear. The available materials, and the corresponding expressions for different properties, are listed in the following subsections.

5.3.1   Ideal solid

Thermal conductivity (W/m·K)

$$1 \times 10^8$$

Density (kg/m³)

$$1 \times 10^8$$

Heat capacity (J/kg·K)

$$1 \times 10^8$$

5.3.2   Copper

Thermal conductivity (W/m·K)

$$398 - 0.0567 * (T - 300)$$

Density (kg/m³)

9000

Heat capacity (J/kg·K)

420

5.3.3   Nickel

Thermal conductivity (W/m·K)

$$\begin{cases} 63.8 + 0.08066 * (631 - T) & \text{if } T < 631 \text{ K} \\ 63.8 + 0.02156 * (T - 631) & \text{if } T \geq 631 \text{ K} \end{cases}$$

Density (kg/m³)

8700

Heat capacity (J/kg·K)

530

5.3.4   Stainless

Thermal conductivity (W/m·K)

$$\left(266800T^{-5.2} + 0.21416T^{-1.6}\right) - 0.25$$

Density (kg/m³)

$$8274.55 - 1055.23\exp\left\{-\left[(T - 273.15 - 2171.05)/2058.08\right]^2\right\}$$

Heat capacity (J/kg·K)

$$\left(1.7054T^{-0.88962}/10^6 + 23324/T^6\right)^{-1/3} + 15/T$$

5.3.5   Molybdenum

Thermal conductivity (W/m·K)

$(33.96 - 0.0095t) - 4.128/10^8 t^2)4.186$

Density (kg/m³) $10868.6 - 2637.52\text{exp}\left\{-\left[(T - 273.15 - 11383.7)/9701.36\right]^2\right\}$

Heat capacity (J/kg·K)

$253.791 + 0.0584 * (T - 273.15) - 2.74 * (T - 273.15)^2/10^6$

5.3.6   Tungsten

Thermal conductivity (W/m·K)

$135.5 + 1.05/10^4/T - 0.023T$

Density (kg/m³)

$19254\left\{1 - 3\left[-8.69/10^5 + 3.83/10^6 (T - 273.15) + 7.92/10^{10} (T - 273.15)^2\right]\right\}$

Heat capacity (J/kg·K)

$135.76\left(1 - 4805/T^2\right) + 0.009T + 2.313T^3/10^9$

5.3.7   Mylar

Thermal conductivity (W/m·K)

$0.11 + 1.7T/10^4$

Density (kg/m³)

$1400 - 0.175T$

Heat capacity (J/kg·K)

$3.7T$

5.3.8   Celcor

Thermal conductivity (W/m·K)

2.5

Density (kg/m³)

2510

Heat capacity (J/kg·K)

$262.5 + 1.864T - 0.001011T^2$

5.3.9   Kapton

Thermal conductivity (W/m·K)

$0.2\left[1 - \text{exp}\left(-T/100\right)\right]$

Density (kg/m³)

$1445 - 0.175T$

Heat capacity (J/kg·K)

$3.7T$

5.3.10 Ceramic (Cordierite)

Thermal conductivity (W/m·K)

2.5

Density (kg/m^3)

2300

Heat capacity (J/kg·K)

900

6 Auxiliary functions

The Auxiliary functions play a vital role in our code. their purpose is to allow system manipulation while maintaining convergence of the shooting method. When "smooth mode" is selected, the auxiliary functions are called for automatically whenever the system is manipulated. however they can be accessed individually by right clicking the buttons or relevant labels.

6.1 ChangeSmooth

This function changes a a system variable smoothly from it's current value to a new value. The shooting algorithm is run on every step, with the converged result from the previous step used as an initial guess for the next step.

The function can also serve an additional purpose: data collection. often it is neccesary to know how changing a certain parameter (e.g. length of one component) influences other parameters (e.g pumped heat). When a parameter is changed, any number of additional parameters can be stored at every step, and the data collected and plotted.

Input Parameters:

Component- The component who's property is being changed. Could be either the system itself (for changing the frequency, mean pressure or initial conditions) or one of the thermoacoustic components.

n:- the number of steps for the change.

Collected parameters:- any parameter to be collected and stored during the run.

Plot: whether or not to plot the parameter after changing.

6.2 ChangeGas

This function changes one of the gases of the working mixture while maintaining guesses and targets. The gas can be either the new inert gas or the new reactive gas.

Input Parameters:

New Gas: The new working gas to be changed to.

Which Gas: whether the changed gas is the inert gas or reactive gas.

n:- the number of steps for the change.

6.3 SwitchMode

This function changes the system's working mode from dry (classical) to wet (phase change) and vice versa.

Input Parameters:

n:- the number of steps for the change.

6.4   InsertSmooth

This function inserts a component into the system smoothly while maintaining guesses and targets. To call it, select smooth mode and drag the component into the system at the correct location.

6.5   RemoveSmooth

This function removes a component from the system smoothly while maintaining guesses and targets. To call it, select smooth mode and drag the component out of the system.

7   Examples

Four example files are supplied along with the installation files. These examples include a dry standing-wave engine (Swift, 1992), a wet standing-wave engine (Brustin et al., 2020), a looped travelling-wave engine (Jin et al., 2017), and a wet standing-wave refrigerator (Yang et al., 2021). Note that the last three systems are illustrated in the article (under peer-review).

8 Tutorial videos

The tutorial videos can be found in xxx.

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