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PC-TAS: A design environment for phase-change and classical thermoacoustic systems

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ABSTRACT

Thermoacoustic technology is a novel approach for high-efficiency, low-cost and environmentally-friendly electricity production, cooling and other applications. In particular, phase-change thermoacoustic conversion is a more recent addition to this field, which is expected to significantly improve the performance of thermoacoustic systems. Here, we present PC-TAS, a tool capable of simulating both phase-change thermoacoustic and classical (no phase change) systems. This tool may be used to investigate how a (phase-change) thermoacoustic system works under steady state by calculating the distributions of acoustic, temperature and species concentration fields. The general model framework is described first, followed by the structure of the code. Next, examples including phase-change and classical thermoacoustic systems are illustrated, and the results are validated against the widely-used software DELTAEC (Ward B et al.. Design environment for low-amplitude thermoa-coustic energy conversion. In: Software users guide. Los Alamos NationalLaboratory; 2008, la-CC-01-13), and against available experimental data. The good agreement indicates that PC-TAS provides a reliable and accessible platform for design and research of thermoacoustic systems, especially for those with phase change.

Code metadata

Current code version	1.01
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-21-00236
Code Ocean compute capsule	https://codeocean.com/capsule/4902048/tree
Legal Code License	BSD-3-Clause
Code versioning system used	none
Software code languages, tools, and services used	MATLAB, MATLAB App Designer
Compilation requirements, operating environments & dependencies	MATLAB application: MATLAB 2020b or newer versions Stand-alone desktop version: MATLAB runtime
Link to developer documentation/manual	https://wetlab.net.technion.ac.il/files/2021/10/users-guide.pdf
Support email for questions	ramong@technion.ac.il

1. Motivation and significance

The interaction of a sound wave with a solid boundary can lead to energy conversion, given proper phasing between heat transfer and the acoustic field. This interaction is known as the thermoacoustic effect, and can be used for converting heat into acoustic power, or for pumping heat by consuming acoustic power [1]. Based on this effect, thermoacoustic devices have been considered as a new generation of heat engines and refrigerators due to the absence of moving parts, the adoption of environmentally-benign working gases and the potential for high efficiency [2]. However, after being studied for more than four decades, the room for further improving the performance through traditional pathways, such as improving acoustics, is becoming increasingly narrow, as clearly seen in travelling-wave devices where the achieved acoustic field is becoming close to ideal

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(i.e., near travelling-wave phase and large acoustic impedance) [3,4]. A promising approach for a breakthrough that significantly improves the performance of thermoacoustic systems is the use of phase-change thermoacoustic conversion [5–10]. In phase-change thermoacoustic devices, the working fluid is a mixture consisting of an "inert" gas and a "reactive" component, which undergoes periodical evaporation and condensation during the oscillation. The presence of phase change increases the energy density of the thermoacoustic process by absorbing and releasing latent heat and increasing the amplitudes of density and velocity oscillations. As a result, the thermoacoustic conversion can be enhanced. This effect has been demonstrated in recent studies of phase-change (or wet) thermoacoustic engines and refrigerators [7–14]. Furthermore, it has been predicted that the phase-change thermoacoustic conversion has the potential to increase the energy density of classical thermoacoustic devices by up to one order of magnitude, with an efficiency above 40% of Carnot limit, especially when working under small temperature differences [9,10].

On the other hand, accurate and cost-effective computational tools (linear-model based tools, for instance) for the simulation of thermoacoustic devices are of crucial importance for research, design and optimization of thermoacoustic systems. However, none of the existing tools can be used to simulate phase-change thermoacoustic systems, hindering the development of this new and promising field.

In this work, we present the physical model, the code structure and the validation of PC-TAS (Phase Change Thermo Acoustic Simulator)—a software for the simulation of thermoacoustic systems, including both phase-change and classical systems. Its graphical interface allows the users to conveniently build virtual thermoacoustic engines or refrigerators. The results of the simulation, including the details of the acoustic field (distributions of pressure and velocity amplitudes), as well as the temperature and concentration fields, can be shown through built-in graphics or exported for further analysis. In this way, the details of a (phase-change) thermoacoustic system can be displayed, helping users to design or analyse a thermoacoustic device.

2. Software description

2.1. Physical model

Thermoacoustic systems typically consist of stacks or regenerators for thermoacoustic conversion, heat exchangers for the input/output of heat, resonators for establishing a proper acoustic field, and acoustic loads/sources for harvesting/supplying acoustic power. Some examples of both the classical (dry) and phase-change (wet) thermoacoustic systems are displayed in Fig. 1. In these systems, the heat and mass transfer of the fluid may generally be described by the continuity equation, Navier–Stokes equations and energy balance equation for the fluid, supplemented by a mass balance for the reactive component, as applicable. Based on the long-wavelength, low amplitude acoustic approximation, the full equations can be simplified into three ODEs. This simplified model was first developed by Raspet et al. [5] and Slaton et al. [6], and later extended by Weltsch et al. [15] and Offner et al. [7] to include other mass-exchange processes (e.g., absorption and adsorption). Here, we use the dimensional versions of the equations derived in Offner et al. [7]:

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

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

$$\frac{dT_m}{dx} = \frac{\dot{H}_2-\frac{1}{2}\Re\left[p_1\widetilde{U}_1\left(1-\frac{\widetilde{F}_\nu-F_\alpha}{(1+Pr)(1+\epsilon_s)\widetilde{F}_\nu}\right)\right]-\dot{m}l_{\mathrm{h}}}{\frac{\rho_m c_p|U_1|^2}{2A_{\mathrm{gas}}\omega(1-Pr)|F_\nu|^2}\Im\left[\frac{(\widetilde{F}_\nu-F_\alpha)[1+\epsilon_s(1-F_\nu)/(1-F_\alpha)]}{(1+Pr)(1+\epsilon_s)}-\widetilde{F}_\nu\right]-\left(A_{\mathrm{gas}}k+A_s k_s\right)}, \tag{3}$$

where p_1 and U_1 are the amplitudes of the oscillating pressure and volumetric velocity, respectively, and T_m and ρ_m denote the mean temperature and density of the mixture, respectively. In addition, a is the speed of sound, c_p the heat capacity, γ the heat capacity ratio, β is the thermal expansion coefficient, R_g is the universal gas constant, ω is the angular frequency. k and k_s denote the thermal conductivity of the gas and solid, respectively, and l_h is the latent heat of the reactive component, A_{gas} and A_s represent the cross-sectional area for gas and solid, respectively, while Pr is the Prandtl number and Sc is the Schmidt number. ϵ_s is a parameter accounting for the finite heat capacity of the solid material, and its expressions for different geometries as used in Ward et al. [16] are adopted. We note that future modification of ϵ_s may be required in the wet-mode calculation, since the influence of phase change on the surface of the solid is currently not considered. The symbol $\Im$ denotes the imaginary part of a complex quantity. $\dot{m}$ is the time-averaged mass flux. The functions $F_n (n = \alpha, \nu, D)$ account for the cross sectional geometry of the system. η_ν and η_D are functions of phase change kinetics, geometry, and the liquid layer's capacity for absorbing additional molecules. Following Offner et al. [7], for evaporation/condensation, they are both assumed to equal 1. C_m is the mean mass fraction of the reactive component. Note that when $C_m = 0$, Eqs. (1) to (3) recover the form of the governing equations for classical thermoacoustic conversion. Therefore, the software can simulate both classical and phase-change systems, although we emphasize its use for the latter. The expressions/values of all the abovementioned parameters can be found in the users' guide.

Eqs. (1) to (3) can describe most of the effects in a thermoacoustic system, but sometimes other effects, including turbulence, heat transfer in heat exchangers, acoustic-electric transduction and lumped compliances, also need to be considered. We follow DELTAEC [16] to address these additional effects, and the details can be found in the user guide.

2.2. Software structure

The code behind the software is based on an object-oriented structure, which ensures the robustness, enhances the re-usability, and enables easy manipulation while constructing a system. Its class hierarchy is displayed in Fig. 2. There are two types of classes derived from the superclass "Component". The first type is the physical classes representing the physical components in a thermoacoustic system (with blue background). We provide six physical classes: the class "Stack&TBT" represents the stack (or regenerator) and the thermal buffer tube; the class "Duct" represents the resonator; the class "HX" represents the heat exchanger; the class "Cone" represents the cone section; the class "Speaker" represents the electric-magnetic transducer; finally,

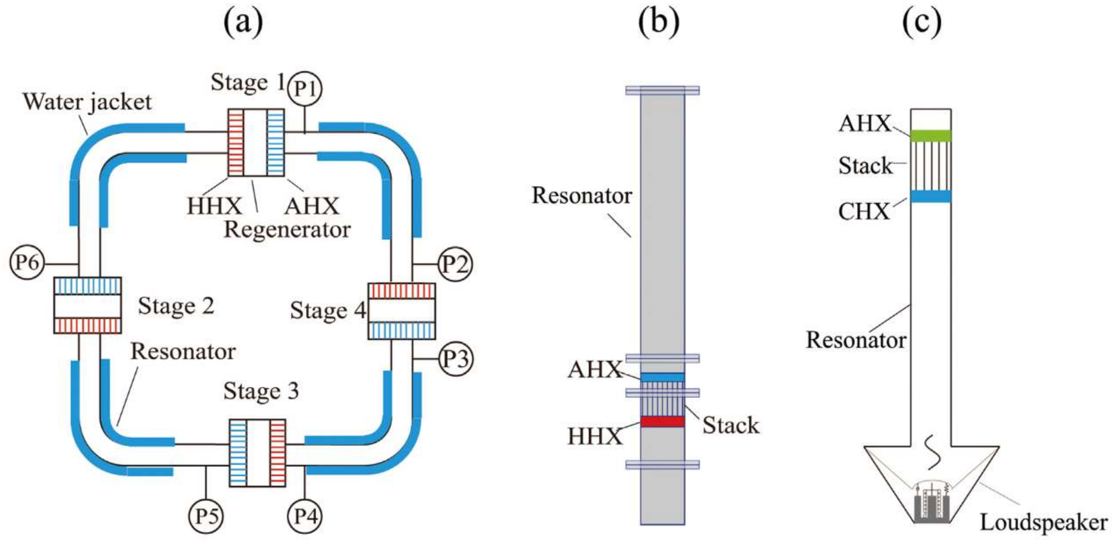

Fig. 1. Some examples of thermoacoustic systems. (a) A dry travelling-wave engine (adapted from Jin et al. [17].) (b) A wet standing-wave engine (adapted from Brustin et al. [18].) (c) A wet standing-wave refrigerator (adapted from Yang et al. [10]). AHX-ambient heat exchanger, HHX-hot heat exchanger, CHX-cold heat exchanger.

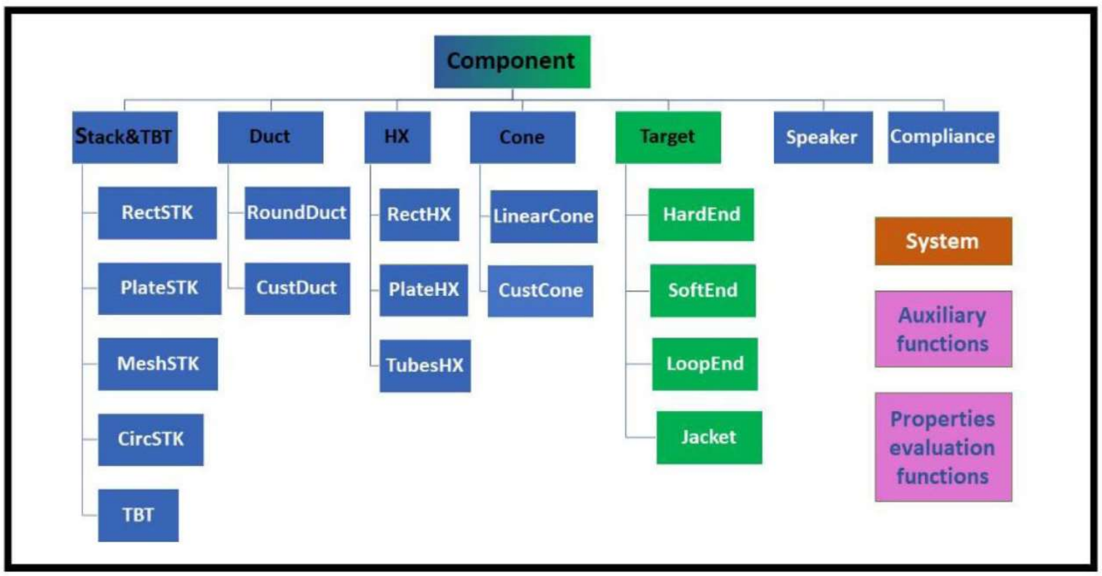

Fig. 2. Class hierarchy of PC-TAS. The superclass "Component" includes all the physical segments of thermoacoustic systems (blue background), as well as targets describing the boundary conditions (green background). The "System" class (orange background) represents the entire system, allowing to combine the different components and run the calculations. Abstract class names are in black text, while implementable class names are in white text. Independent functions (blue text, pink background) work for mixture and solid properties evaluation. Auxiliary functions serve for system modification and investigation. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the class "Compliance" represents any form of acoustic compliance, e.g., a large volume. The subdivisions under some of these classes represent the corresponding components with specific geometries. Each component obtains the values of the pressure amplitude, volumetric velocity amplitude, temperature and total power at its inlet.

The second class, under the superclass "Component", is the "Target" class. Targets are non-physical classes (i.e., not representing actual segments of the system), representing boundary conditions, which we refer to as "targets" for the shooting algorithm. We provide four predefined targets: The "HardEnd", which generally represents the boundary of a solid termination, targets the value of velocity to be zero. The "SoftEnd", which generally represents the boundary of a large acoustic compliance, targets the pressure amplitude to be zero. The "LoopEnd", often used in a looped configuration, imposes periodic boundary conditions. The "Jacket", used at the transition between an isolated component and a jacketed component, targets $\dot{H}_2 = \dot{E}_2$ and thus prevents nonphysical discontinuity in the total power.

The "System" class represents the entire thermoacoustic system built by the user with the physical and logical components. When the virtual system is run, all components are calculated sequentially, yielding the distributions of the pressure and volumetric velocity amplitudes, the temperature, the mass flux and the acoustic power, with each component receiving its input parameters from the previous one.

The "Property evaluation functions" are used for obtaining the transport properties of the working gas mixture, as well as the properties of the solid, with the input of the mean temperature, concentration (as applicable) and pressure.

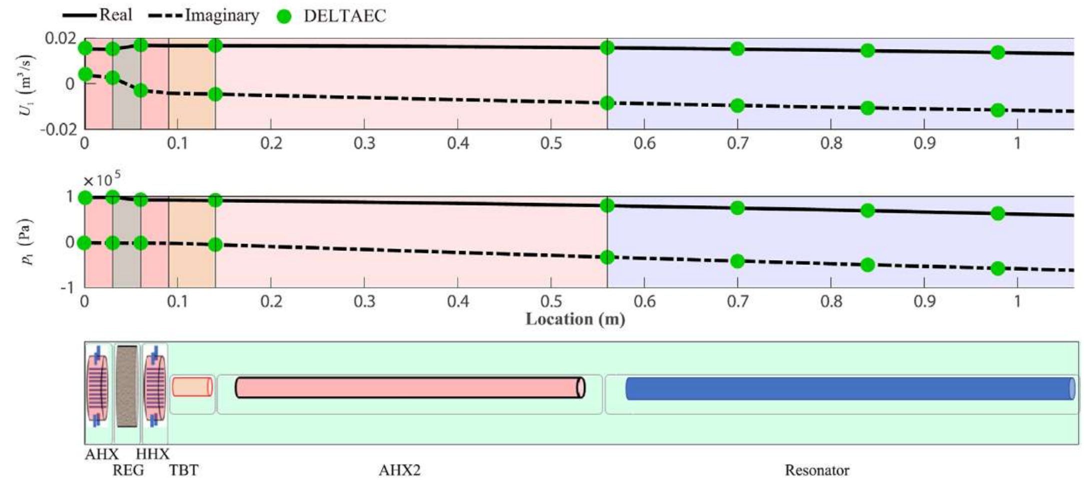

Fig. 3. Distributions of the volumetric velocity amplitude (top) and the pressure amplitude (middle) in the travelling-Wave engine designed by Jin et al. [17]. Schematic of the engine generated by PC-TAS is displayed at the bottom. Note that the resonator is only partly shown, because it is too long.

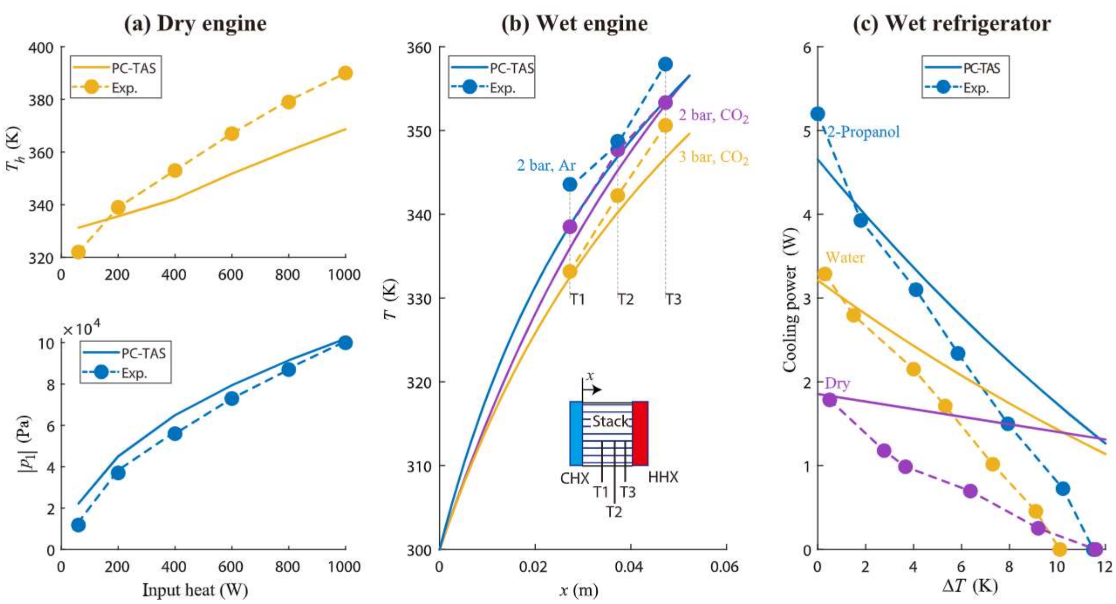

Fig. 4. Validations of PC-TAS against experimental data from the three systems presented in Fig. 1. (a) The validation of the classical (dry) travelling-wave engine developed by Jin et al. [17]. The comparison in both the hot end temperature T_h (top) and the pressure amplitude $|p_1|$ (bottom) with different input heat are presented. (b) The comparison of the temperature distribution along the stack in the phase change (wet) standing-wave engine designed by Brustin et al. [18]. (c) The comparison between calculated and measured cooling power with different temperature differences ΔT, in a phase-change (wet) standing-wave refrigerator developed by Yang et al. [10].

The "Auxiliary functions" serve for system modification and investigation after the virtual system is built. Specifically, the function "ChangeSmooth" changes the geometrical and physical parameters of the system (i.e working frequency, length of a component); "ChangeGas" changes the working fluid; "SwitchMode" switches a phase-change system into a classical system (no phase change) or vice versa; "InsertSmooth" and "RemoveSmooth" are used to insert or remove a physical component into a system, respectively.

3. Validation and illustrative examples

To illustrate the quality of the simulation by PC-TAS, in what follows, we compare the obtained results with those from a widely-used software for classical (dry) thermoacoustic systems, and with experimental data of both phase-change (wet) and classical (dry) systems. All of the examples are provided along with the installation files.

3.1. Validation against DELTAEC

We first validate the dry-mode performance of PC-TAS against the software DELTAEC, which has been widely used for simulation of dry thermoacoustics [1,16,17]. The travelling-wave engine developed by Jin et al. [17], whose schematic can be seen Fig. 1(a), is used as the example. Only a quarter of the system was simulated due to the symmetry of the configuration. As can be seen in Fig. 3, the results of both pressure amplitude p_1 and volumetric velocity amplitude U_1 are almost identical with those from DELTAEC, proving that the dry-mode performance of PC-TAS is reliable.

3.2. Validation against experiments

Next, we compare the calculated results against the experimental data of the engine by Jin et al. [17], in terms of the distributions of pressure amplitude and hot temperature with different input heat, as shown in Fig. 4(a). The calculated and experimental pressure amplitudes are in good agreement in both trends and magnitudes; the calculated temperatures show errors up to 10%. One reason for the deviation is Gedeon streaming, which exists in the looped configuration and may distort the temperature field significantly [1,19], but is not included in the simulation due to the lack of reliable equations. In addition, the abrupt changes in cross-sectional area between the resonator and the regenerator may cause local radial effects, which are unaccounted for and so may also introduce errors.

To validate the wet-mode simulation, which is a unique feature of PC-TAS, we demonstrate two examples and the corresponding comparisons with experimental data. The first case is a wet, standing-wave engine developed by Brustin et al. [18] (see Fig. 1(b)). The calculated and measured temperature profiles along the stack are shown in Fig. 4(b) respectively. In all the three operating conditions, the calculated temperature agrees well with the experimental data in trend, albeit slightly lower (within 5 K). The second case is a phase-change standing-wave refrigerator developed by Yang et al. [10] (see Fig. 1(c)). The calculated and experimental results are compared in terms of cooling power versus temperature difference between the two heat exchangers, with three reactive components. As can be seen in Fig. 4(c), a good agreement is obtained for small temperature differences, and the deviations become increasingly large with the rise of temperature difference. This is mainly attributed to the heat leakage in the stack section, which is ignored in the software and become more severe with the increased temperature difference.

4. Impact

Phase-change thermoacoustics is a promising approach for efficient, clean and cost-effective energy conversion. PC-TAS provides a convenient and reliable tool for simulations of Thermoacoustic devices. The accessibility of this tool will help users understand the related mechanisms, as well as design and analyse phase-change thermoacoustic devices. For example, theoretical analysis for phase-change thermoacoustic systems in Tsuda and Ueda [11,12] and Yang et al. [9,10] can be done efficiently.

Thanks to the user-friendly graphical interface, users with limited knowledge on thermoacoustics can perform the simulation with little time investment, which will encourage researchers who may have been hindered by thermoacoustic theory that seems to be arcane, especially with phase change, to enter this promising field.

Furthermore, the presented software may still be used for the simulations of classical thermoacoustic devices, with the same accuracy as its predecessor, DELTAEC, but extendable to new features arising in the more recent research of thermoacoustics (e.g., the bi-directional turbine [20], piezoelectric transducer [21], triboelectric transducer [22], etc.). These have been scheduled in the near future versions of PC-TAS, although users are also encouraged to add these by themselves.

5. Conclusions

In this work, we present the software PC-TAS—a simulation tool for phase-change and classical thermoacoustic systems (including but not limited to engines and heat pumps). The physical model and code structure have been described. Furthermore, the illustrative examples demonstrate that it is a reliable and convenient tool for the research of thermoacoustics. In particular, we highlight its most important attributes, as follows:

- Added physics—the ability to simulate phase-change thermoacoustic conversion.
- An object-oriented code structure, enabling easy manipulation.
- A user-friendly graphical interface, allowing convenient system design by dragging and dropping virtual components.

Some limitations of PC-TAS should be mentioned here. First, the code solves the set of equations derived within the framework of linear theory, and so assumes one-dimensional, single frequency oscillations. These assumptions are generally valid for low-amplitude oscillations ($p_1 \ll p_m$), both in the wet and dry modes. Higher-order effects such as the streaming, additional harmonics as well as spatial effects (e.g. at transition points, near end terminations etc.), are unaccounted for, potentially resulting in significant deviations at higher amplitudes. Second, the ideal-gas model and the kinetic model for estimating the transport properties of the mixture would also benefit from additional validation. Finally, in the wet mode, PC-TAS assumes that the mixture is in contact with a liquid layer of the reactive component, which indicates permanent wetting, or, alternatively, sorption to/from a layer with sufficient material capacity. In cases where such conditions are not maintained, some error in the calculations is also expected. These additional effects constitute future extensions of the theory and, eventually, the software.

Conflict of interest

We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

A User manual, source files and installation files are all included in supplementary material, as of the time of publication. The latest version of all the above, as well as video tutorials, are available at https://wetlab.net.technion.ac.il/pc-tas/

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