

TSS-ARKS

Thermal Safety Series - Advanced Reaction Kinetics Simulation **Software**



User's Guide

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1 Introduction

Simple Vent Sizing is the program module form TSS-ARKS software series which supports the simple methods of vent sizing for reacting systems. This module can can be called from ARKS AC or ARKS HA as the server for vent sizing analyses. When working with ARKS AC calculations are based on processed data of adiabatic test. When Vent Sizing module is called from under ARKS HA it uses fata of simulation of an industrial reactor thus providing more relevant results.

Simple Vent Sizing allows the choice between two methods of of calculation of flow through vent line:

the method introduced by the part of the standard ISO 4126-10 Safety devices for protection against
excessive pressure — Part 10: Sizing of safety valves for gas/liquid two-phase flow that is related to
reacting system. This standard in its turn is based on modification of Leung methods for calculation of
the required flow rate to be discharged

J.C. Leung, "Simplified Vent Sizing Equations for Emergency Relief Requirements in Reactors and Storage Vessels", AICHE-Journal, Vol. 32, No. 10, 1986, 1622/1634 (see https://www.fauske.com/sites/default/files/

Simplified Vent Sizing Equations for Emergency Relief REquirements in Reactors and Storage Vessels.pdf), and

J.C. Leung, "Venting of Runaway Reaction with Gas Generation, AICHE-Journal, May 1992,

and "Omega" method for calculation of the dischargeable mass flux through a safety valve

(" A generalized correlation for one-component homogeneous equilibrium ?ashing choked ?ow". AIChE -Journal Vol. 32, No.101986:1743–1746).

See also J. Etchelis and J. Wilday, Workbool for Chemical Reactor Relief System Sizing (http://www.iomosaic.com/diersweb/docs/crr98136a.pdf)

• the J.C. Leung's method.

Essential feature of the Standard is that the corrections have been introduced in the original method for taking into account nonequilibrium of the two-phase flow when calculating the flow rate (discharge) through a safety valve whereas the original "Omega" method by Dr. Leung was derived for homogeneous equilibrium two-phase flow model.

It should be emphasized that the corrections introduced by the ISO-4126-10:2010 are still not well grounded physically and don't take into account such important vaporization characteristics as the number of vaporization nuclei and existing bubbles, surface tension, thermal conductivity coefficient for a liquid; it doesn't take into account the possibility of slipping of phases. Therefore the results of the Standard-based calculations of two-phase flow should be considered with due care.

Notes

- 1. In general, the nonequilibrium correction makes the method not enough conservative in contrast with the homogeneous equilibrium model. Bearing in mind that the simplified methods for the calculation of the required flow rate to be discharged by themselves represent quite rough approximation we cannot recommend to use this correction.
- 2. Comparison with the calculations based on more precise models that simulate runaway (methods introduced by SuperChems (IoMosaic), BST (CISP) and some others) shows that the Leung method, being applied to pure vapor system and quasi-single component mixture (when mixture species have comparable properties) provides reasonable accuracy if the difference between the set pressure and overpressure is not big.
- 3. In the case of gas and hybrid systems all the simplified methods often give essentially overstated size of safety devices.
- 4. When calculating the required flow rate to be discharged along the Leung method **Simple Vent Sizing** applies the formulas from the ISO 4126:10 standard that don't take into account decrease of the mixture volume during the discharge till attaining the maximal pressure. It results in more conservative estimates than the original Leung method.

2 Getting Started

Simple Vent Sizing can be be invoked from the Analysis panel of ARKS AC after extracting necessary data from the experimental pressure curve (use the ARKS AC Help or ARKS AC User's guide in ARKS AC/DOC folder).

Before launching Vent one should:

- 1. Select the appropriate type of the system. 3 types are supported Pure gas, Gassy or Vapor one.
- Pure gas means that the overall (aggregate) gas generation is calculated on the basis of the total
 pressure; therefore it includes pad gas (inert gas in an adiabatic bomb) and vapors. It represents the most
 conservative case as amount of gas is overestimated.
- Gassy system. In this case amount of gas is calculated on the basis of pressure of gaseous products. In general case vent sizing takes into account both gases and vapors thus representing the hybrid system.
- Vapor system is appropriate choice when pressure of vapors essentially exceeds pressure of gaseous products and; therefore, gases can be neglected.

More details can be found in the ARKS AC User's guide in ARKS AC/DOC folder.

2. Define set pressure Po and maximal allowed accumulation pressure Pmaa.

The Main window appears.

To quit Simple Vent Sizing, do one of the following:

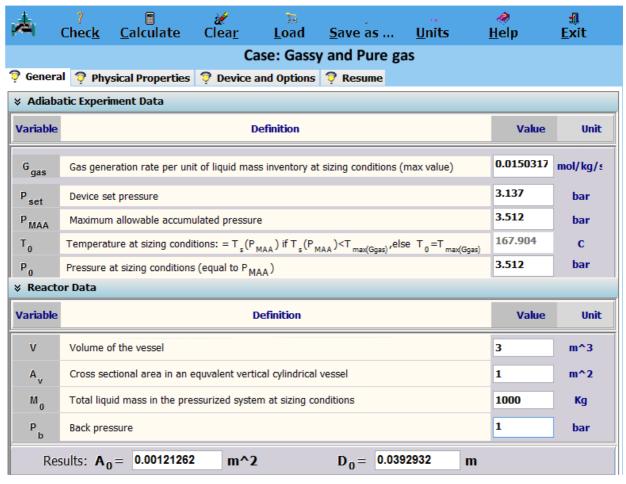
- From the toolbar of the main window, choose Exit.
- Click the Close button [x] at the right upper corner of the main window.
- Double-click at the left upper corner of the main window caption.

2.1 Main Window of Vent Sysing Module

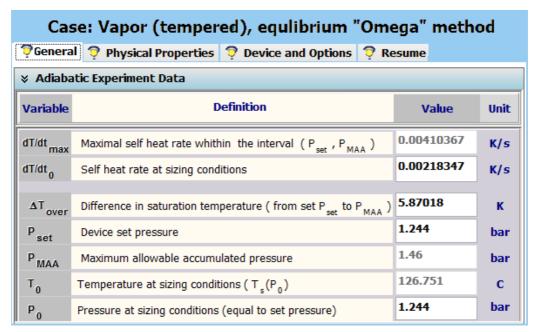
The main window has 4 pages - General, Physical properties> Device and Options and Resume (see details below).

When the Vent module is launched the main window opens on the General page. Its layout differs depending on the system type you selected.

For Pure gas and gassy system is as follows.



For vapor system the Definition table is different:



The main window has the **Tool bar**, the **Data panel** with four pages (see Tabs in Figure) and the **Results** panel on the bottom

The Tool bar contains the following controls:

Check	button; click it to verify data consistence. If all the data on certain data page are consistent
	the corresponding tab is marked by the
	green light 💸, otherwise it is marked by the red light 🧝

Calculate button runs vent sizing

Clear button is used when you want to clear all the data loaded

Load button opens the Load data dialog which allows selecting and loading necessary part of a Vent sizing project previously saved into the Vent sizing projects data base.

Save as button opens the Save as dialog to save a Vent sizing project into the Vent sizing projects data base.

Units button opens the Customizing Units of Measurement dialog which allows adjustment of units.

Help button activates the Simple Vent Sizing Help

Exit button closes the module

The Tabs allow access to the following data pages:

General page with Adiabatic Experimental Data and Reactor Data;

Physical Properties page consists of two tables for defining Properties of liquid and gas at set conditions
and Data for checking limitations of the method table

Device and Options page consists of two tables for defining Device Data and Options

Resume page which displays the error and warning messages

Note

Every data table has the caption. By clicking the caption you can expand and collapse the table

3 Preparing Initial Data

The following data must be defined for calculation:

- data from adiabatic experiment
- Reactor data
- · Safety device data
- Properties of Liquid and Gas mixtures
- Data for checking limitations of the method

Furthermore, certain Options are available for adjustment.

The set of data represents the Vent sizing project that can be

- saved into the Vent sizing data base, or
- · loaded from this database.

This chapter explains how to implement all these actions.

3.1 Defining the Adiabatic Experiment's Data

The General page shows the Table Adiabatic Experiment Data.

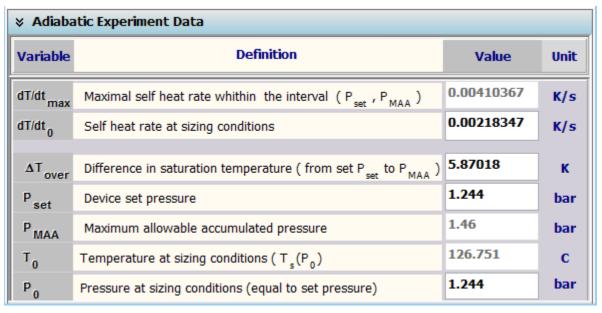
It contents depends on the system's type you selected.

- Vapor (tempered) system, when gas generation is negligible. In this case for quasi one component system liquid temperature strictly depends on pressure. When you assign set pressure and maximum allowable pressure, take into account that In this case 30% overpressure is recommended: (P_{MAA}/P₀-1 < 0.3);
- 2. Pure Gas system. In this case it is supposed that total pressure in the adiabatic bomb has been created only by gaseous reaction products. In accordance with this assumption self-heat doesn't depend on pressure in the system. In this case the gas production rate is the maximal rate expected under adiabatic conditions. By default the experimental temperature at the moment when gas generation is maximal is selected as the set temperature. This is the more appropriate choice that can be recommend.
- 3. Gassy or Hybrid system is a fluid system, which at sizing conditions exhibits characteristics of both tempered and gassy systems to a significant extent. This represents the most complex case. Depending on the balance of pressure and temperature the same reactive mixture can behave as gassy or vapor system.
 - when working pressure is high, temperature can rise for a long time while pressure remains practically
 constant due to periodical opening of safety valve as long as vapor pressure is essentially smaller than
 the set pressure and additional vapor flow rate is small.
 - when saturated vapor pressure becomes big enough and represents sufficient part of the set pressure, vapor flow may become dominant. Due to limitations of the vent sizing method it cannot properly take into account the following features of hybrid system: reduction of maximum temperature level due to evaporation, and effect of subcooling of liquid in the vessel (relative to saturation temperature) on the discharge; therefore size of safety device can be overestimated..

If **Vent Sizing** module was invoked from ARKS AC then all the Data of Adiabatic Experiment are imported from ARKS AC and are not editable.

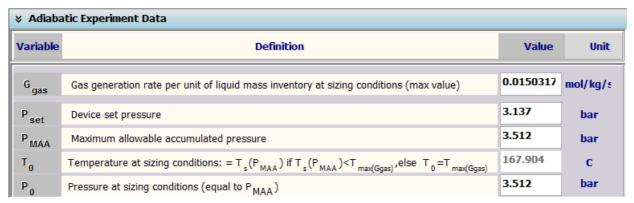
3.1.1 Adiabatic Experimental Data for Vapor Case

Sizing temperature and pressure correspond to device set pressure. All data at Adiabatic Experiment Data panel are transmitted from client software ARKS AC.



3.1.2 Adiabatic Experimental Data for Gassy (Hybrid) Case

The Adiabatic Experiment Data panel for Gassy (Hybrid) and Pure gas systems is shown below.



All data are transmitted from client software ARKS AC. If evaporation can be neglected, then the mixture experimental temperature at the moment of maximum gas generation can be used as the sizing temperature and sizing pressure is a certain value less than P_{MAA} . If data regarding vapor generation is presented (molar heat of evaporation L_{sm} and equilibrium vapor pressure $P_s(T)$) the system is identified as Hybrid. Since the liquid temperature normally cannot substantially exceed the boiling point at a given pressure, it is recommended to fix the value of sizing temperature T_0 as $T_s(P_{MAA})$. Such the values are retrieved from experimental data and assigned by default. Values of dT/dt_{max} and G_{gas} are used during the whole runaway.

Note

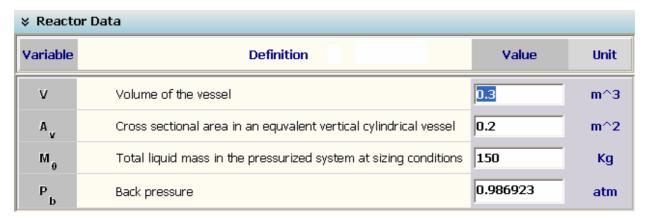
In the general case gas generation by a reaction can be accompanied by vaporization. The feature of such a system is that temperature rise may not be inhibited by evaporation and is less dependent on pressure. Unfortunately, standard ISO 4126-10 (2010) does not contain physically sound formulas for modeliing hybrid situation where vapor and gas generation both play a significant role. It results in possible overestimation of vent sizing up to a discouraging degree. Properties of gas at sizing conditions are undefined due to unknown composition and temperature at sizing pressure. Therefore, for a hybrid system, we recommend using the ARKS CK software for creation of concentration reaction kinetics followed by using the ARKS BST program and it's Vent Sizing procedure. Less preferably, but also possible to use the ARKS FK program to construct formal kinetics. If vaporization can be neglected, the standard ISO 4126-10 formulas for gas discharge can be applied.

3.1.3 Adiabatic Experimental Data for Pure Gas Case

When the Pure Gas system has been chosen, it means that all the pressure in a vessel is assumed to be pressure of gaseous products. Apparently it overstates amount of gases as in fact it includes also vapors. The **Adiabatic Experiment Data** panel for **Pure Gas** case is identical to **Gassy** (Hybrid) case.

3.2 Defining the Reactor Data

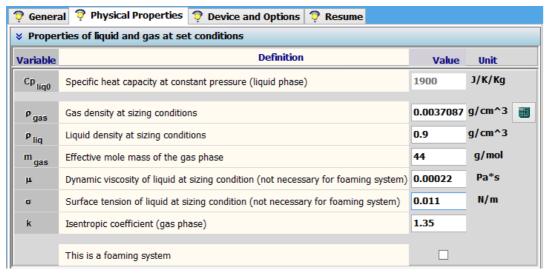
The **Reactor Data** allows defining parameters of the reactor - its volume, mass of the mixture, back pressure, etc.



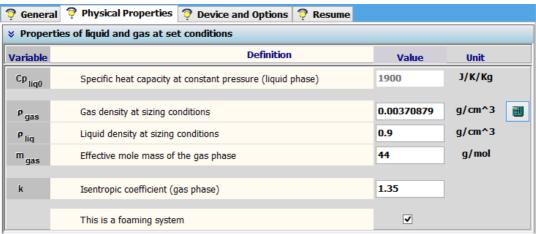
3.3 Defining Properties of Liquid and Gas

The **Physical property** page is used for defining Properties of Liquid and Gas Phase at the Sizing Conditions. Contents of the page depends on the system type and some other adjustments.

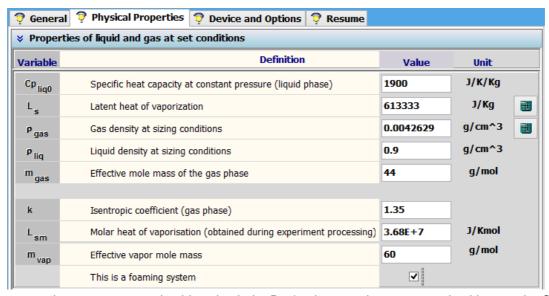
For the Pure gas system and Gassy system without taking into account vapors the page appears as shown in Fig. below.



On can choose between foamy and non-foamy system by checking/unchecking the **This is a foaming system** check box. If the foaming system has been selected the unnecessary data lines Dynamic viscosity and Surface tension would be hidden as shown below

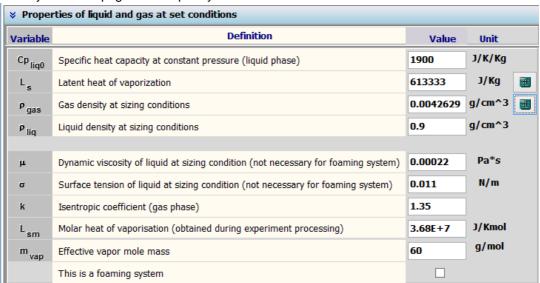


When Gassy system has been chosen and vapors should be taken into account (the Hybrid system is to be considered) then the page appearance changes:



To take vapors into account one should uncheck the Don't take vapor into account checkbox on the Options page if it had been checked.

Finally, the layout of the page for a Vapor system is as follows:



When the Vent module is launched from under ARKS AC some properties data are transferred and are displayed, namely:

- Specific heat capacity of liquid;
- Molar vaporization heat L_{sm} is determined in ARKS AC when vapor pressure is approximated by the Antoine/August equation (see ARKS AC User guide).

To calculate vaporization heat per unit of mass L_s first define the effective molar mass of vapors. The Calculator button \overline{m} appears on the right of the Ls edit, click it to calculate.

Gas density can be calculated applying ideal gas law after defining the effective molar mass of gas. As soon as it is defined the Calculator button appears on the right of the Gas density edit, click it to calculate. When you have chosen the Vapor system, vapor density will be calculated instead after defining effective molar mass of vapors.

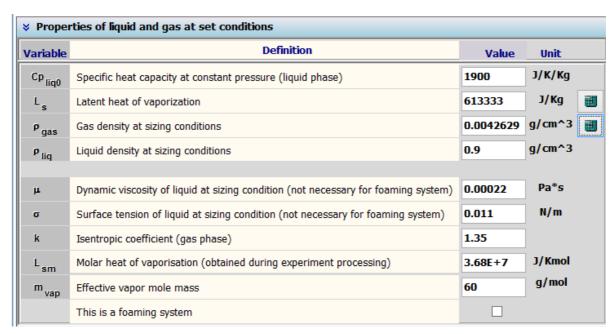
Note

Sometimes necessary data regarding liquid and gas properties are not immediately available. Therefore Vent goes with some exemplary data presented in the Exemplary properties data for Vent. xlsx file which can be found in the ARKS AC/DOC folder.

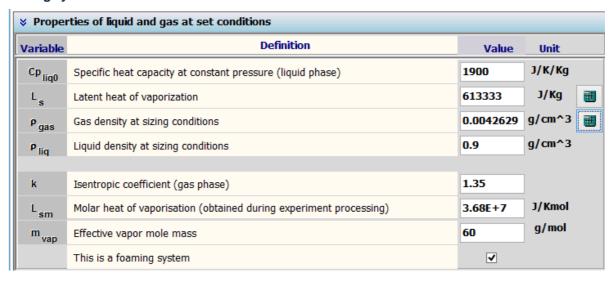
3.3.1 Physical Property Data for Vapor Case

Here is the example of properties for the Vapor system for two cases - foaming and non-foaming (see also Defining Properties of Liquid and Gas)

Non-foaming system:

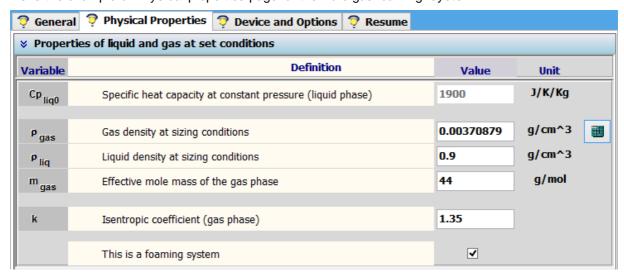


Foaming system:



3.3.2 Physical Properties Data for Pure Gas Case

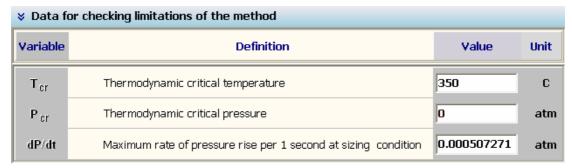
This is the example of Physical properties page for the Pure gas foaming system.



In this case data are prepared in a special way - gas production is calculated from the total pressure and includes vapors; therefore information about vapor pressure (heat of vaporization) is not transferred in the Vent module. That is why the properties page doesn't display the parameters related to vapors (latent heat, molar mass of vapors). Moreover the checkbox **Don't take vapor into account** on the Options page is checked and blocked.

3.4 Defining Data for Checking method's Limitations

This page contains data necessary for checking limitations of the methods:



First two values correspond to the limitations of the method for calculating the flashing two-phase mass flux in safety valves and limitations of the method for calculating the required mass flow rate to be discharged:

The maximum rate of pressure rise dP/dt should also be defined.

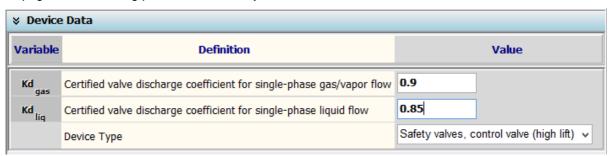
When checking the limitations the value of self-heating rate (see Defining the Adiabatic Experiment Data) is also taking into account.

Note

Limitations are not inspected if the checkbox Check method limitations on page Options is not checked. In this case all the edits of the page are disabled.

3.5 Defining Device Data

This page allows defining parameters of safety device.



Values of Kd_{gas} and Kd_{liq} should not exceed 1, in addition Kd_{gas} cannot be bigger than Kd_{liq} .

Note

Typical value of $Kd_{gas} = 0.971$, $Kd_{liq} = 0.65$ (API RP 520 recommendations). It is also recommended the value = 0.85 for two-phase flow.

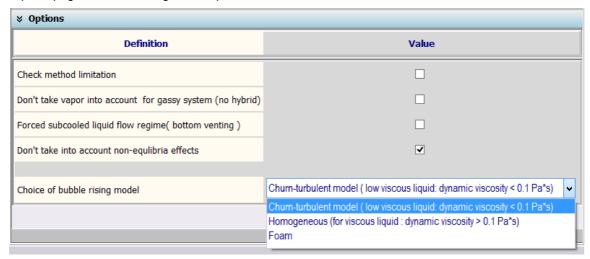
Device type is used when the boiling delay factor is calculated (see coefficient a in formula 35a of ISO 4126-10) . For equilibrium (Leung) case device type is not taken into account.

Three device' groups are considered:

- Safety valves, control valve (high lift);
- Long nozzles, orifice with large area ratios;
- Orifices, control valves, short nozzles.

3.6 Options

The Option page allows defining some options for calculation.



Check method limitation check-box; if it is not checked data for checking limitations of the methods will be ignored and validation will not be performed.

Don't take vapor into account for gassy system (no hybrid) check-box; if it has been checked then additional vapor mass flow rate (see formula 10 of ISO 4126-10 standard) will not be taken into account during calculation.

Forced subcooled liquid flow regime (bottom venting) checkbox; if it has been checked then only liquid flow through safety device will be taken into account.

Don't take into account non-equilibria effect check-box; if it has been checked then non-equilibrium correction will be ignored during calculation (boiling delay factor will be equal to 1). This case is equivalent to the Leung method, therefore even if you want to use Leung method you can easily switch to this method by checking this checkbox.

Choice of bubble rising model lisbox allows the choice one of 3 models of bubble rising in reactor:

- Churn-turbulent model (low viscous liquid: dynamic viscosity < 0.1 Pa*s)
- Homogeneous (for viscous liquid: dynamic viscosity > 0.1 Pa*s
- Foam; selection of this model is equivalent to checking the checkbox **This is foaming system** check-box on the **Properties** ... page; therefore it will be checked automatically.

3.7 Load data from data base

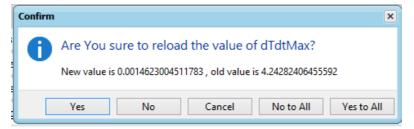
The **Load** option allows selecting and loading necessary part of a Vent sizing project previously saved into the Vent sizing projects data base.

Press the Load button from the Main Window toolbar. The Load dialog appears



Use the check-boxes to select which components of the project to load and press the **Load** button. The conventional Open dialog appears; choose the path to the project files, select necessary project file and open it.

When the project is loaded the program will ask to confirm replacement of the existing data with data from the project to be loaded:



One can confirm or refuse replacement of specific data, all the data set or cancel the load.

Note

It may happen that the project you selected doesn't contain some components you indicated in the Load dialog. In this case you will have to define deficient data manually

3.8 Save data to data base

The **Vent Sizing** module has its own data base for storing vent project. You can save certain parts of the current project for further use by using the **Save as** option. To do it press the **Save as...** button from toolbar of the Main Window. The Save as dialog appears:



You can save all the data set or certain components. Use the corresponding checkboxes to define composition of a project to be saved, then press the **Save** button. The standard Windows Save dialog appears. Select the path to the place where you want to store the project, then define the project name in the File name edit box, and press **Save**.

The project file will be saved with the SVP (Sizing Vent Project) extension. It is a text file that can be renamed, moved, copied and deleted in a conventional way.

4 Checking Data

By pressing the **Check** button you can verify data consistence.

If all the data on certain data page are consistent the corresponding tab is marked by the green light 🔊



otherwise it is marked by the red light

When a new project is started or opened all the tabs are marked by the yellow light 👽

If some inconsistency had been found or mistakes made the corresponding info (errors and warnings) appears on the **Resume** page so that data that require correction can be easily identified.

5 Getting Results

When all the data are consistent press the **Calculate** button of the Main Window toolbar to calculate the size of a safety device.

The results - vent area Ao and throat diameter Do will appear in the bottom panel of the Main window.

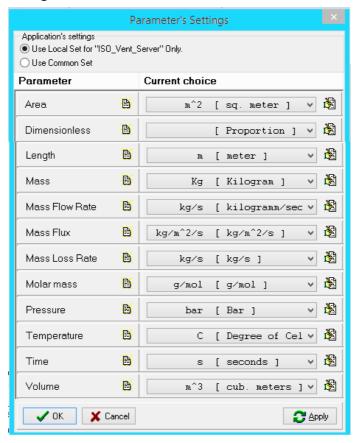
Note

The results of vent sizing accompanied with main ifo about the project will be included in the ARKS AC Word report after closing the module (see ARKS AC User's Guide in the ARKS AC/DOC folder)

6 Customizing Units of Measurement

The **Vent Sizing** module has a useful feature for adjustment of units of measurement to make input of data and their representation more convenient. The standard (SI) and some non-standard units are allowed. The user can also register custom units.

All the adjustments are made in a special **Parameters setting** dialog which appears after clicking the **Units** button of the**Vent Sizing** main window toolbar.



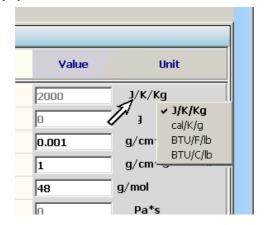
After completing units adjustment click **Apply** or **Ok** to put the changes into force. If you click **Ok**, the dialog will be closed; if you click **Apply**, it remains active. To cancel the changes, click **Cancel**.

Notes

- 1. Unit settings has no effect on data representation in property database tables.
- 2. If you choose **Use Local Set for ISO_Vent only** the settings will have effect on the Vent module only. If you choose **Use Common Set** the settings will have effect on all the TSS ARKS applications installed that support this advanced feature.

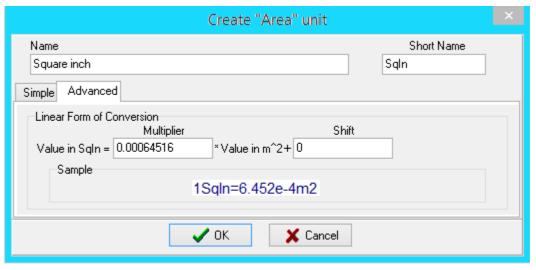
6.1 Changing the Unit for a Quantity

To change the unit for a quantity, you should choose this unit from the listbox beside the quantity name.



6.2 Registering a Custom Unit

To register a custom unit for a quantity, click Create new unit button beside the quantity name. In the dialog-box appeared, type the unit name and short name in the corresponding fields. Then enter conversion coefficients (coefficients of the linear dependence to express the new unit in terms of the standard unit) and click **Ok**. The new unit will appear in the unit list.



Note

Only linear unit conversion is available

6.3 Editing a Registered Unit

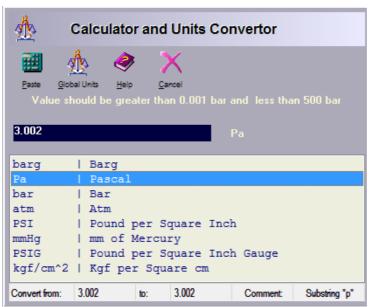
To edit an existing custom unit, choose this unit from the listbox beside the quantity name and click the Edit/View current unit button on the right. In the dialog appeared, edit the unit name, short name and conversion coefficients in the corresponding fields. Then click **Close**.



6.4 Input of values in different units

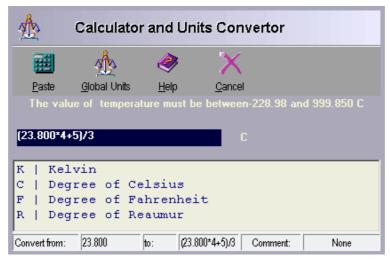
If you don't want to change unit performance you can entry data in any appropriate units other than the current one. In any field expecting the input of a dimensional value, you can quickly convert the value entered in various units into the currently used units.

Enter a value in the desired unit. Then press a key corresponding to the initial letter of the unit name (e.g. "p" for Pascal, or "C" for degree of Celsius). The following window appears:



If the name of the desired unit is not selected in the list, select it. Finally press **Enter** key (or click **Paste** button). The converter window closes, and the entered value will be substituted with equivalent one expressed in the currently set units. For example, if the current unit for temperature is degrees of Celsius, you can type 70F, and finally the value of 21.121C will be shown in the changed field of dimensional edit box or dimensional grid cell.

You can use this calculator for simple arithmetic computation.



To start the arithmetic calculation when calculator is not yet opened, you can type in any field expecting the input of a dimensional value a symbol of arithmetic operator for nonempty field. If the field is empty press the key =.

There are the list of arithmetic operators:

Operator	Meaning	Example
+	addition	1+2
-	subtraction	10.3-0.5
1	division	10/3
*	multiplication	3*5
۸	exponentiation	2^4
Pi	π	Pi/2
(left parenthesis	(1+Pi/3)*4
)	right parenthesis	
exp()	exponent function	exp(Pi/4)

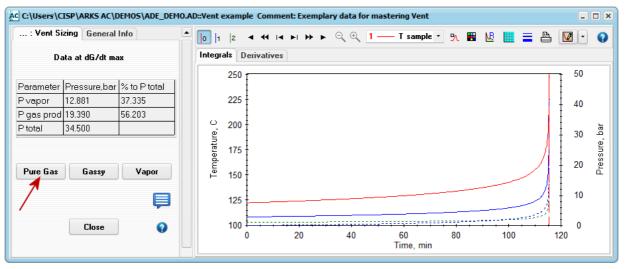
6.5 Unregistering Custom Units

To unregister a custom unit for a quantity, choose this unit from the listbox beside the quantity name and click the Edit/View current unit button on the right. In the dialog appeared, click **Unregister**. After your confirmation the custom unit will be removed from the list.

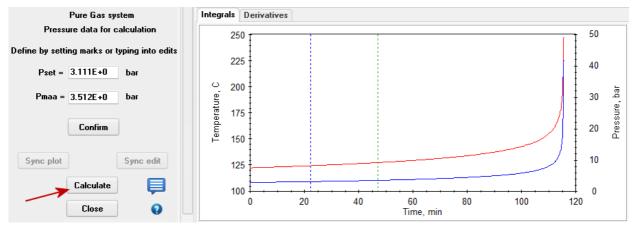
7 Example of using Vent

The following example illustrates how to use Vent. It is based on the exemplary data Vent example from the ARKS AC/DEMOS/ADE_demo.ad data volume so that you can reproduce all the steps by yourself. It will help in mastering software.

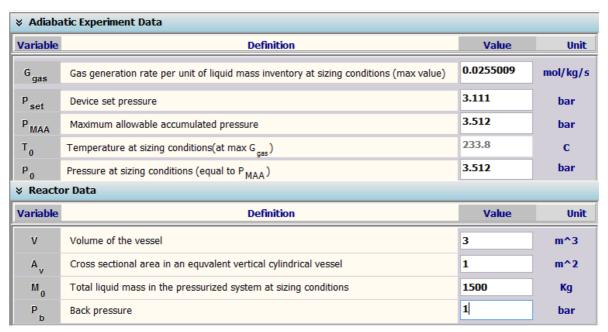
- Open the Vent example dataset. Original data have been processed and corrected on thermal inertia; therefore they are ready for vent sizing. Go to Vent sizing command of the ARKS AC instrumental panel. The dialog allows choosing the system type.
- 2. The first variant is Pure gas, which provides the most conservative estimates



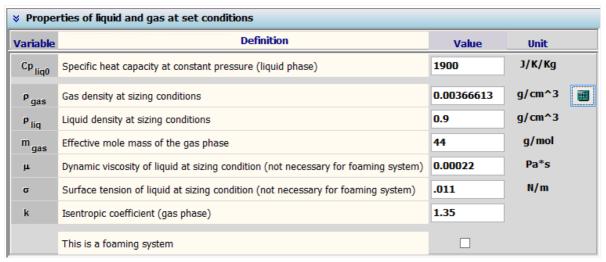
- 3. Press the Pure Gas button
- 4. Now you should define set pressure Po and maximal allowed accumulated pressure Pmaa. To do this set Mark 1 and Mark 2 and press Sync. Edit. The Calculate button becomes active. Press it



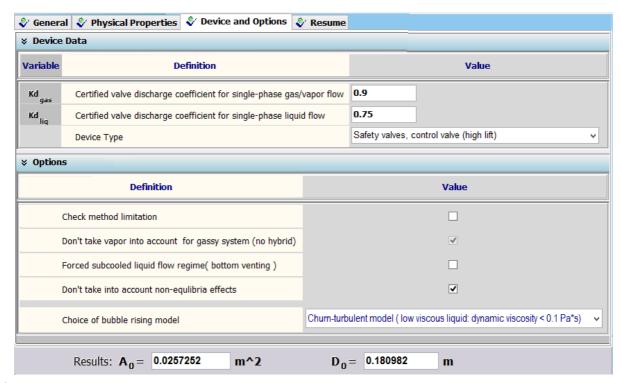
5. The Vent main window opens. The first page displays experimental data transferred from the ARKS AC. Define the reactor's parameters.



6. Go to Physical properties page and define necessary properties. At first it is assumed that the system is non foaming and it will be single-phase gas discharge.



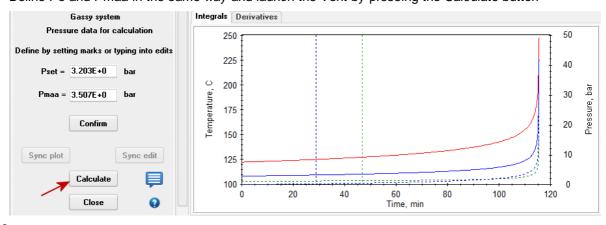
7. Define the parameters of a safety device, Check whether data have been defined properly, and run calculation



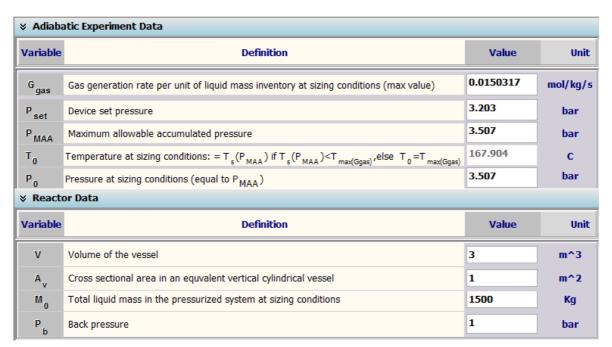
8. Close the Vent module. you will be returned to the ARKS AC. Close the dialog for selecting pressures. You will be redirected to the system type selection step. Select Gassy system



9. Define Po and Pmaa in the same way and launch the Vent by pressing the Calculate button

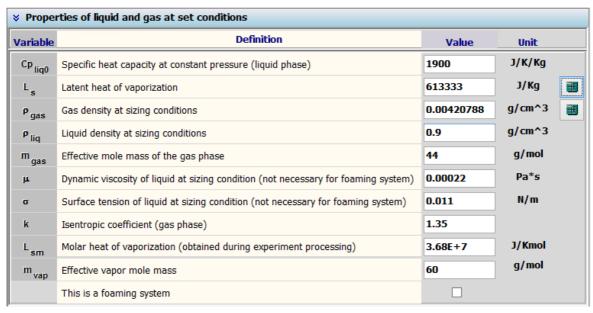


10. The Adiabatic data page is as follows

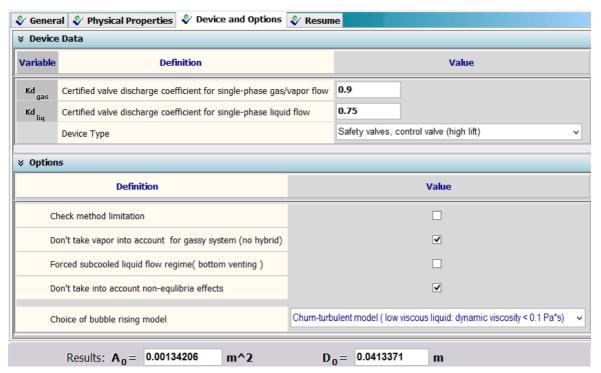


Note that maximal gas generation rate calculated without vapors is lower than in case of the Pure gas system.

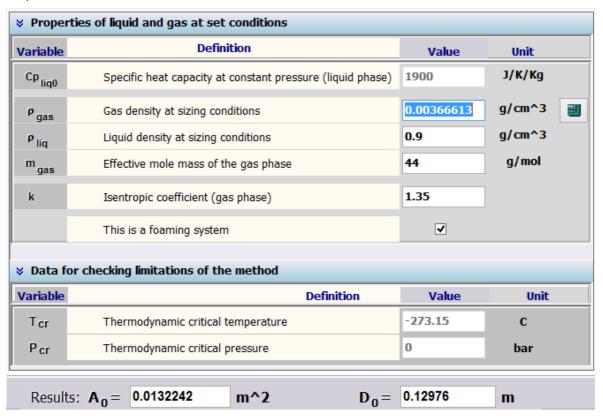
11. This time the Properties page displays more information because there are data regarding vaporization and by default the system is treated as the hybrid one.



12. By refusing to take into account vapor the system will be considered and gassy. With the same parameters of the safety device the throat diameter is about 4.5 times smaller than for the Pure gas system because of essentially smaller amount of gaseous products. As in previous case the discharge is single-phase gaseous.



13. Now select the foaming system to reveal the effect of two-phase flow in the required size. Check the checkbox This is a foaming system and run calculation. This time the diameter is 3 times bigger than in the previous case.



You can try other variants, for instance to check whether taking vapors into account will affect the results for foaming and non-foaming systems or try to consider the system as Vapor one.

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