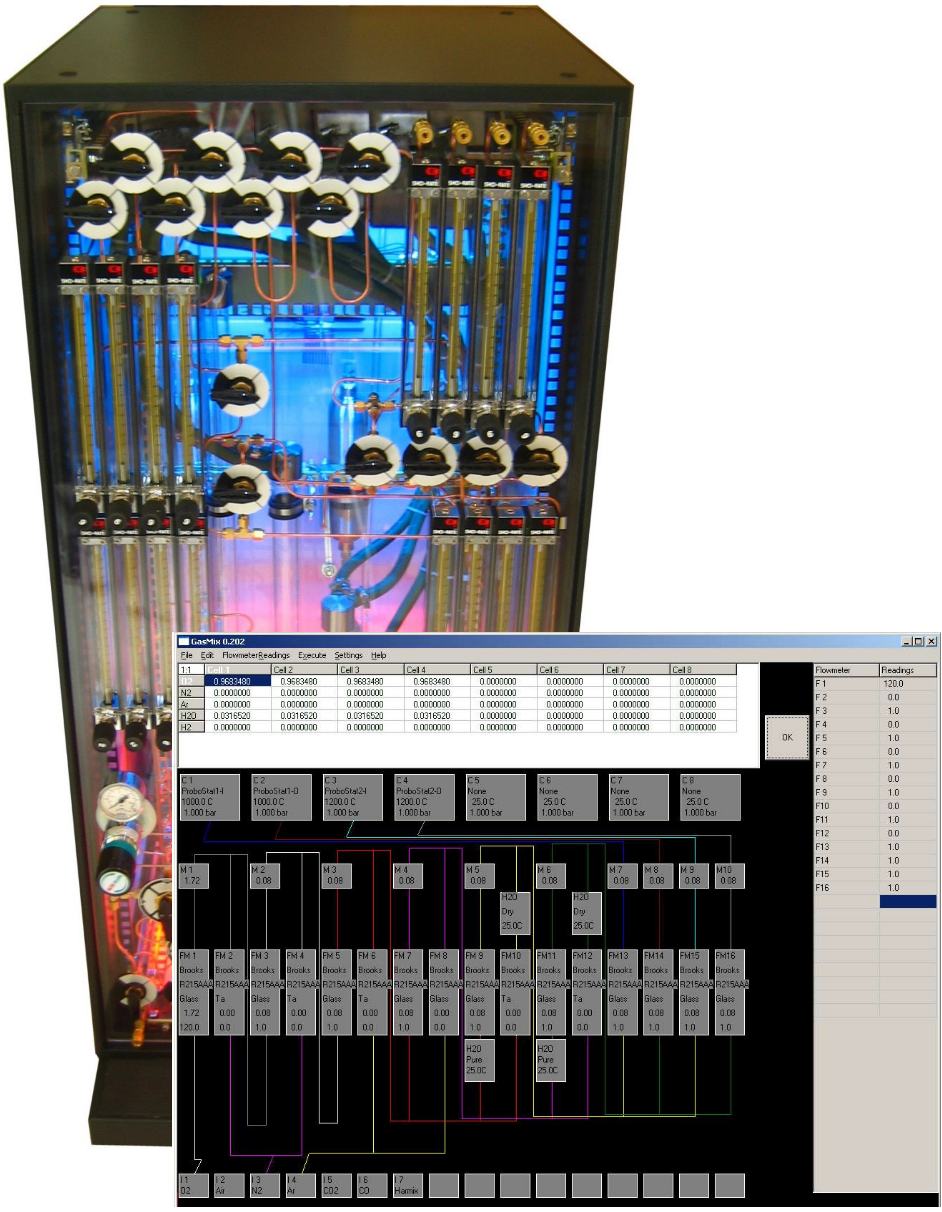
GasMix



User Manual

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GasMix software

1.1 *Introduction*

1.1.1 What is GasMix?

The GasMix program is software for calculating gas mixing ratios and also equilibrium compositions resulting from gas mixers such as the ProGasMix. However, the program has flexibility of configuration and use that makes it useful also for other gas mixing applications.

1.1.2 History of GasMix – past and present

The GasMix for Windows is a development from the GasMix program written by Truls Norby for HPBASIC computers in the 1980s and used in his group at University of Oslo till this date for calculating gas mixtures on gas mixers analogous to the ProGasMix.

At present, the new GasMix software that you here are reading about and perhaps are trying out, is in its early development. This means that

- Some functions of the program aren't implemented yet.
- The chance of bugs and incorrect calculations is considerable.
- User friendliness and ease as well as screen information are not optimised.
- This manual is in the midst of being written; it may have parts where the intended sections are missing or uncompleted. There may be minor errors in references to menus etc. in the program.
- My apologies! Your comfort is that it can only get better and that it is free! Look for updates at http://folk.uio.no/trulsn/gasmix.htm

1.1.3 GasMix emulates but does not control your mixer

To avoid any misunderstanding: GasMix emulates the physical gas mixer and makes calculations based on the readings taken from the mixer. It is however not physically connected to the mixer in any way, it does not communicate with the mixer and it does not control the mixer in any way.

1.2 *Installation and startup*

1.2.1 GasMix package

The GasMix software package consists of 6 files:

GasMix.exe The program itself

GasMix Manual.pdf This manual (may also be integrated in another manual, e.g. a ProGasMix Manual.pdf)

Four parameter files, containing data for GasMix definition and calibration:

GasMix.inp	Input gases definitions
GasMix.mix	Mixer setup
GasMix.cal	Flowmeter calibration
GasMix.cel	Output cell setup

1.2.2 Copy to directory c:\Program Files\Gasmix\

The package may be installed anywhere on your Windows computer. However, we suggest that you install it a directory

c:\Program Files\GasMix\

If it does not exist, create it, and copy all GasMix package files there.

1.2.3 Make a shortcut

Point at the Gasmix.exe icon. Right-click and Create Shortcut. Move the shortcut to your desktop or elsewhere. Rename it e.g. “Shortcut to GasMix”.

1.2.4 Start and run the program: GasMix.exe

Start the program GasMix.exe from the shortcut icon or in any other way. Go to Section 1.3 for a quick-start introduction and tutorial or to Section 1.5 for a more thorough treatment of the GasMix definitions, capabilities, and operation.

1.2.5 Updates

If you later download or otherwise receive updates of the program, manual or parameter files, simply overwrite the existing ones. Consider, however, to make a copy of all existing files in a separate directory in case the original or edited parameter data will be needed or the new program version does not work on your computer for some reason.

1.3 GasMix quick-start and tutorial

This section intends to give the user a fast introduction to the GasMix software and practice in using it. For deeper definitions, specifications and explanation, refer to Section 1.5.

1.3.1 Start and run the program: gasmix.exe

Start the program GasMix.exe from the shortcut icon or in any other way.

1.3.2 Overview of the gas mixer and GasMix display

At the bottom of the display are a row of small boxes, each representing an Input gas. Typical Input gases are the pure gases or mixtures that come from bottles or lines of gas in your laboratory, e.g. O_2, Air, N_2, Ar, 5% H_2 in Ar.

Next – at middle height of the display - comes a row of vertical rectangles, representing the Flowmeters. Some of the Flowmeters may be fed from the Input gases, and this is then illustrated by coloured connecting lines – one colour for each Input gas.

Above the flowmeters gas lines show how the flowmeters are connected to form Mixtures. Each Mixture has a colour, and there is one small boxes attached to the Mixture line above the first flowmeter connected to that Mixture.

Additional small boxes directly below or above a flowmeter represent stages for fixing the partial pressure of some component, normally H_2O (wetting or drying stages).

On the top you find rectangles representing your measurement or reaction chambers, here called Output cells, for which temperature and total pressure can be set so as to allow calculation of equilibrium partial pressures.

The right hand side of the window is reserved for tables in use during editing and data entry. Moreover, results of mixing and equilibrium calculations will appear on the top of the window.

During editing of calibration curves also parts of the mixer schematic temporarily becomes covered with tables and graphs.

1.3.3 Run a simple session with typical actions

Load a set of parameter files to define everything. In the menus, go to File menu and select Open All. A file dialog allows you to find the location of the setup files (*.MIX, *.CAL, *.CEL, and *INP). Click on one of them, and all (up to four) that are found with the same first part of the filename are loaded.

If the mixer that appears has something in at least one of the input mixture boxes at the bottom, and something in at least one flowmeter box at middle height, and lines making some connections between input mixtures and flowmeters and further to an output cell at the top, the mixer appears to be configured with a real or tutoral example and should be ready to do something. In that case, leave the Edit menu unused for the moment.

Select FlowmeterReadings in the top menu. A table appears where you edit the readings of flowmeters. If the readings look sensible, leave them, or change one just for the test. Or you may enter for instance 3 as a reading for all flowmeters. Press the OK button. The edited readings should now be visible at the bottom of the flowmeter boxes.

Select Execute in the top menu. Now the program makes all calculations of mixtures and displays them in a table for output cells and partial pressures of gas species.

In the Settings menu change the display from linear to logarithmic.

There is also a possibility to change between room temperature contents and equilibrium values. Equilibrium calculations are not correctly operating yet.

You may now go on doing more things, or minimise the program, or exit from File, Exit.

1.4 GasMix operations in more detail

1.4.1 Edit the input mixtures

With input mixtures is meant what you may often call gases – the gases that are supplied to the mixer from pressured bottles or lines. They are actually generally mixtures, firstly because some of them are, such as air or hydrogen that is diluted with an inert gas to make it explosion safe. Secondly, even simple gases contain impurities, and these may be entered into the input gas and makes it a mixture.

Start editing input mixtures by Edit, InputMixtures.

Next to the table that appears, the name of the input mixture s entered in the separate window. This name has no meaning other than to identify the input mixture. If it is oxygen 99.99 %, then you may for instance call it O2 or Oxygen or O2-4N.

In the table itself, enter the names of the gas species and their content pairwise in the two columns. The name must be exactly the same as the one used in the calibration curves, and normally also exactly the same as the program uses for equilibrium calculations. Typically valid names are O2, N2, Ar, H2 and H2O. Names should here not reflect a mixture. (For instance Air is not meaningful here.)

The gases contained in the input mixture may be entered in any order.

The units of content may be any as long as it is consistent for each input mixture. The program only uses the partial pressure calculated as the content divided by the total content.

Note that water (H2O) may be entered as an impurity in an input mixture, but water as such is normally not entered as an input mixture – it comes in via humidification stages.

1.4.2 Edit the flowmeters and gas mixer configuration

Start editing flowmeters and their configuration by Edit, Flowmeters.

Go to the appropriate flowmeter by using the up/down controls. Edit the table. Remember to press OK before proceeding to the next flowmeter. The mixer layout scheme changes only upon pressing the OK button.

All information regarding the make, type, and float of a flowmeter is edited here. Remember that exact spelling is required for the calibration curves to recognise the flowmeter. (The actual flow reading is not edited here, but in a special table accessed directly from the FlowmeterReadings menu point.)

Moreover, it is specified what gas mixture the flowmeter is supplied with. This is done by writing I # (where # is a number) for Input Mixtures, and M # for mixed Mixtures.

It is also specified which mixture the flowmeter feeds to, numbered simply from 1 to 16. Note that the box specifying the mixture and its total flow is placed after the first flowmeter only (for practical reasons) while it actually signifies all the flowmeters going into that mixture.

Finally, you can here specify Fixed gas pressure units – normally simply humidification or drying units. For this, the gas species to be fixated, the method, and the temperature (when relevant) are specified. In addition, the use of the unit can be switched between Yes and No, and you specify whether it is placed before or after a flowmeter.

For humidification, let the gas be H2O and the method be Pure or KBr, and set the temperature to that of the humidification step – equal to the room temperature if you have no special reading or thermostat. For drying, let the method be Dry.

Note that when you press OK to confirm the changes made to a flowmeter, the mixer scheme changes on the screen.

1.4.3 Edit the output cells

Start editing flowmeters and their configuration by Edit, OutputCells.

Select which mixture to feed the cell.

Give the impurity/background levels of gas species you consider appropriate to add to the final gas mixture fed to the cell. The source of these may be typical leakages, permeable gas line hoses, permeable high temperature cell wall materials, desorption, or impurities in the input mixtures not specified other places. The gases species you can add impurity or background levels to are O2, H2O, H2, and N2. For single walled high temperature cells we suggest O2 = 1E-5 (10 ppm) and H2O = 3E-5 (30 ppm) as realistic settings (with H2 and N2 zero).

Select the cell's temperature and pressure if used for equilibrium calculations..

Press OK to confirm the changes.

1.4.4 Edit the calibration curves

GasMix can store up to 1000 flowmeter calibration curves.

Each curve can hold up to 20 data pairs (reading, flow).

All curves must have the same unit for readings. The default – and the unit used in the calibration curves supplied as standard with GasMix – is litres/hour (l/h). Litres here of refers to standard litres (1 atm, 25 °C).

Start an editing session from Edit, Calibration.

The numerical data are entered in the right hand table.

The data MUST be entered in increasing order of Reading. You do not need to use all 20 rows, but the last rows not used must hold only 0,0.

In running the program, readings below the lowest or above the highest valid calibration point are rejected.

The first entry may have a reading of 0, but 0 is anyway always interpreted as zero flow. Any value larger than zero is then interpreted in the normal manner.

If the lowest reading is larger than 1 (e.g. 2) then 1 is given a special meaning, namely to represent the maximum flow. The use of this will be dealt with later on.

You may enter data manually one by one, or you can copy them via the clipboard for instance from Excel. In order to do this, first go to Excel and mark and Copy a section, e.g. the Readings column. Then go to GasMix and press the first cell, then mark all cell in the range you need while holding the Shift key down. Then Right-click inside this range and select Extract from Clipboard.

As you make the calibration curve, check that it looks as expected from the plot that is displayed based on the numbers you enter.

For each calibration curve filled with numbers you must press the OK button to store the data in memory, otherwise the entered numbers are lost. (This is a safety against unintended data entry in established curves.)

The data specifying the flowmeter and conditions for each calibration curve is entered in the left hand side table. Note that the texts entered must be accurately the same as those used for flowmeters are gas species. A misprint means that the program will not recognise the fit of the calibration curve to the flowmeter or gas.

In this table, you can enter data for several curves, but you must press the OK button in order to store the changes in memory. If you go to another operation without pressing OK, the changes are lost.

1.4.5 Edit the flowmeter readings

The flowmeter readings are entered from FlowmeterReadings. Press OK to confirm.

1.4.6 Execute the calculations

Select Execute to do all calculations throughout the mixer. The result is shown in a table where all gas species appear for all Output Cells.

The composition of a mixture is not shown unless the mixture is routed to an output cell.

1.4.7 Settings: Change the display of the output

In the Settings menu you can change between linear and logarithmic display of the gas partial pressures of the mixtures; lin/log toggle.

Moreover, you can select whether the room temperature mixture as fed to the output cell or the equilibrium composition is displayed. The equilibrium display will show only species well defined by their thermodynamics in the program and where the required chemical elements are all present in the mixture fed to the cell. The equilibrium option is not operative yet, and you will only get a warning if you try it.

1.4.8 Error messages

There is a field for warnings and error messages – in red at the bottom of the screen.

1.4.9 Display

You may drag and resize the GasMix window, and maximise/minimise it. In some cases, resizing is a way to refresh the GasMix display if parts are not showing.

If you cannot see all items on screen, it is possible that your screen has a too small resolution. This is mostly a problem with video projectors or small laptops or old computers.

1.5 GasMix technical reference

1.5.1 GasMix capabilities and definitions

The GasMix program comprises a number of components and connections between them, to be described below.

Those that are user editable are accessed through the Edit menu.

1.5.1.1 Gas species

A number of gas species (atoms or molecules) are predefined in the program. They are identified by their chemical formulae: H2, N2, O2, Ar, H2O, CO, CO2, etc. Thermodynamic parameters of formation are connected with these species. These definitions and parameters can not be edited by the user.

1.5.1.2 Input Gases

Up to 16 input gases can be named and defined by the user, corresponding to the gases connected to the inputs of the mixer. Each input gas is actually a mixture of gas species, and the definition is simply a fractional content of the gas species.

The definitions of the input gases can be edited via Edit, Input Gases.

The definitions of the input gases can be stored in files of type *.inp via the File menu and submenus.

1.5.1.3 Flowmeters and mixer configuration

Up to 16 flowmeters can be defined by the user. They are supposedly rotameters and thus identified by their make, model, tube size, and float material, but the make, model, and size can also be used to identify any other type of flowmeter. The definitions of the flowmeter will enable the program to find a suitable calibration curve when the flow is to be calculated.

Each flowmeter can be configured so as to feed any of 16 Mixtures. Further, each flowmeter can be configured so as to be fed from any of the Input Gases or Mixtures.

Each flowmeter can be configured with a gas fixing stage before it or after it. A gas fixing stage fixes the partial pressure of one gas component. Usually, this is a stage for H2O which wets or dries the gas to a certain level. Various ways of operation and calculation can be set, and the temperature of operation also enters.

All these definitions set up the overall connection and mixing scheme of the mixer. The connections are shown graphically on the program screen.

The definitions of the flowmeters, fixing stages, and connections of the mixer can be edited via Edit, Flowmeters.

The definitions of the flowmeters, fixing stages, and connections of the mixer can be stored in files of type *.mix via the File menu and submenus.

1.5.1.4 Calibration curves

Up to 1000 flowmeter calibration curves can be held by the program. They can be entered in any order. They are marked with the flowmeter name, tube size, float material, gas, individual flowmeter, temperature, and pressure that the calibration is valid for. Further, each curve contains up to 20 data points. The program selects the best curve available for any flow calculation.

The calibration curves can be entered or edited via Edit, Calibration.

The calibration curves can be stored in files of type *.cal via the File menu and submenus.

1.5.1.5 Output Cells

Up to 8 output cells may be defined, normally the measurement cells at high temperatures to which gas mixtures are routed and for which equilibria are calculated. The cell can be assigned a gas mixture, total pressure, and temperature. In addition, leakages of H2, H2O, and O2 can be set that will be added to the Gas Mixture arriving.

The definitions of the output cells can be edited via Edit, Output Cells.

The definitions of the output cells can be stored in files of type *.cel via the File menu and submenus.

1.5.2 Parameter files

1.5.2.1 File definitions

The GasMix parameters are stored in four types of files according to the part of the mixer and parameters affected. The types have indicative extensions:

*.inp	Input gas definitions
*.mix	Mixer configuration
*.cal	Flowmeter calibration curves
*.cel	Output cells

1.5.2.2 File operations

The File menu allows the user to open or save files individually. They may then have individual names. Alternatively, they may all be opened or saved in one operation using one and the same name for all.

If one chooses the Open, Save, or Save As options, then a second level allows the selection of operation on one of the Input Gas, Flowmeters (Mixer), Calibration, or Output Cell parameter file. In this way, files with different names may be used for the different parameter sections.

If one chooses Open All, Save All, or Save All As, the operation will affect all four types and they will all address files by one and the same name (except the extension). In this way, entire sets of parameters may be opened or saved more easily.

1.5.3 Calculations

1.5.3.1 Flow of a mixture of gas species through a flowmeter

When a mixture is passed through a flowmeter, the program calculates the flow of each gas species as if it was alone. Then its contribution to the total flow is obtained by multiplication by the partial pressure of the gas. By summation, the total flow is obtained. (There are other and more correct ways of doing this, and these may be implemented in future versions.)

Finally, each gas species gets a partial flow by multiplying the total flow by its partial pressure, and this flow is added to the total flow of the mixture.

It may be noted that a minor component of a gas in this way will be carried onwards by the mixture and would be carried onwards also in the calculations of its partial flow even if this species was not specifically calibrated for and therefore did not get a flow assigned to in the calculation of its contribution to the total flow. However, the way GasMix works, any gas will have a partial flow contribution calculated, using another gas' calibration curve if necessary.

1.5.3.2 Flow of a single gas species through a flowmeter

When the calibration curve is selected the flow of each gas species is calculated from the flowmeter reading and that curve by using a Lagrange interpolation routine.

Readings above the maximum calibration point are not accepted.

Readings below the minimum calibration point are not accepted, with the following exceptions:

The reading 0 (zero) always returns zero flow, even if the extrapolation of the curve gives another value or even if the calibration curve contains the reading 0 as the first entry and the flow associated with it is not zero.

If the minimum reading of the calibration curve is bigger than 1 (one), then the reading 1 is taken to mean the same as the maximum reading. The experienced user can use this for fast entry of readings in parts of the mixer where the actual flow does not matter (no mixing) and it is desirable to just tell the program that gas is running in plenty through the flowmeter.

1.5.3.3 Selection of a calibration curve

The conversion of a flowmeter into a flow requires a calibration curve. The program can hold a large number of calibration curves, and attempts to find the one best suited. At present the algorithm used is the following: The program looks for matching flowmeter make, flowmeter type, float type, gas species, and actual flowmeter. The one with the closest match is chosen. Normally, with standard curves, it will be easy to achieve the first four. To get the fifth it is assumed that you will have made individual curves for individual flowmeters of your mixer.

In future versions of the program it is planned to make the selection more advanced and safer, and to display and verify the selection. Moreover, more advanced manners of obtaining flows of mixtures instead of individual gas species may require different selection criteria.

1.5.3.4 Making mixtures

The partial flows from all flowmeters connected to a Mixture are calculated and added. When all are done, the program divides the individual partial flow of each species with the total flow to obtain the fractional content. If the total pressure is one, the fractional content will correspond to the partial pressure.

1.5.3.5 Fixation of a gas species

When a gas mixture passes a fixation stage, e.g. a wetting or drying stage, the new mixture is calculated according to the following principles:

Before the fixation stage, each gas i has a partial pressure $p_{i,b}$ and the sum of all these is $P_{tot,b}$. After the fixation stage, gas j has had its partial pressure changed from $p_{j,b}$ to $p_{j,a}$. This change may be positive (as in a wetting stage) or negative (as in a drying stage). All the other gases $i \neq j$ will have to share a corresponding decrease or increase in partial pressure, so as to arrive at a sum of the partial pressures $p_{i,a}$ of all gases i corresponding to the total pressure after the stage, $P_{tot,a}$.

If the total pressure is the same both before and after the fixation stage, the partial pressures after the fixation are

$$p_{j,a} \qquad \text{and} \qquad p_{i\neq j,a} = p_{i,b}\frac{P_{tot,a} - p_{j,a}}{P_{tot,b} - p_{j,b}}$$

If the total pressure is unity, as in the present version of GasMix, then this simplifies further into

$$p_{j,a} \qquad \text{and} \qquad p_{i\neq j,a} = p_{i,b}\frac{1 - p_{j,a}}{1 - p_{j,b}}$$

If the fixation stage is inserted before a flowmeter, the new composition is first set, and the flow then calculated using the composition with the calibration of the flowmeter to obtain the total and partial flows.

If the fixation stage is inserted after a flowmeter, the new post-fixation composition of the fixated gas and its new partial flow is calculated, and the new total flow and individual composition of each of the other species are calculated based on the increase or decrease in content of the fixated gas. The formulae used for the composition is the same as used above for pre-flowmeter fixation.

1.5.3.6 Calculations of fixed pressures for various gases and methods

The fixed pressure of water over pure water H_2O (method “Pure”) is calculated with the Goff-Gratch equation, with temperature as input.

The fixed pressure of water over a saturated solution of KBr(aq) (method “KBr”) is taken as 84 % of that calculated by the Goff-Gratch equation. This percentage is specified in the CRC Handbook for 20 °C.

The pressure of water over a drying or getter stage (method “Dry” or “Getter”) is set to zero.

The pressure over pure heavy water D_2O is calculated from the 5th order polynomial formula

pD_2O (kPa) = 0.413333333 + 0.046428671*t + 0.000936772*t^2 + 2.85781e-05*t^3 + 2.5e-07*t^4 + 2.82051e-09*t^5

where t is the temperature in degrees Celsius. The curve is based on a fit using TableCurve 2D to values taken from the CRC Handbook[1].

The pressure over D_2O saturated with KBr is tentatively calculated as 84 % of that over pure D_2O.

The pressure of oxygen over a getter stage (method “Getter”) is set to zero.

The Method names are case insensitive.

1.5.4 Definitions of arrays and indexing used in the program (mainly for programmers)

1.5.4.1 Chemical Elements

The elements are numbered and named according to their atomic number and chemical formula. For instance, hydrogen is 1, H, helium is 2, He, etc.

Deuterium is given the number 122 and formula D, and tritium is given the number 123 and the formula T. No other isotopes are handled as such.

1.5.4.2 Compounds and gases

GasMix operates with predefined **compounds**, for which thermodynamic data are stored and their elemental compositions are defined. They are used in calculations of equilibria. They are indexed by an arbitrary number and identified by their chemical formulae. Any well-defined single phase can be what is here called a compound. Examples comprise monoatomic elemental gases (He, Ar), molecular elemental gases (H2, O2, O3, N2), gaseous compounds (CO, CO2, H2O), and condensed phases such as solid graphite (C).

GasMix furthermore operates with **gases**. These are gaseous species – in one sense the same as gaseous compounds. However, they need not in principle be defined thermodynamically – it is more important in the first instance that the flowmeters are well calibrated for them in order to obtain correct mixing ratios. If equilibria are required however, only gases corresponding to a defined compound (as above) can be properly split into the proper amount of defined elements. The remaining will enter as inert.

1.5.4.3 Mixtures

GasMix stores gas mixtures in a number of arrays, depending on where in the mixing and calculation process they are:

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1 *Handbook of Chemistry and Physics*, 73rd Edition, Lide, D.R. Ed.; CRC Press: Boca Raton 1992; Chapter 6, pg. 10

The InputMixtures array hold all input mixtures – they can be opened from and saved to *.INP files. They can be edited by the user. They are copied into the Mixtures array when a calculation is initiated.

The Mixtures array is an array that holds input mixtures and mixed mixtures alike. It is rearranged in the course of mixing so that all mixtures have the same order of gases. The Mixtures feed the flowmeters and the output cells. The Mixtures array holds only room temperature mixtures, it does not contain equilibrated mixtures.

CompBuffer is a temporary buffer array for the gas species and is used during the calculations of partial flows and setting of fixed gas for each individual flowmeter.

The CellMixturesRT array is similar to the other mixtures, but holds the room temperature mixtures in the output cells. It is copied from the Mixtures array after completion of all calculations in the mixer, and in addition gets the leakages of the gases specified for the individual cell.

There are additionally arrays for equilibrium calculations and equilibrium pressures. These have CellMixturesRT as input and will be described when the equilibrium part is operative.