# **RPA-C**

## **RPA-C v.2 API for Scilab**

## **Table of Contents**

Configuration of environment	6
Using the API	6
Components	6
Configuration API	7
ConstructConfigFile	7
ConfigFile_read	7
ConfigFile_write	7
ConfigFile_fromString	8
ConfigFile_toString	8
ConfigFile_getName	9
ConfigFile_setName	9
ConfigFile_getInfo	9
ConfigFile_setInfo	9
ConfigFile_getGeneralOptions	10
GeneralOptions_isMultiphase	
GeneralOptions_setMultiphase	10
GeneralOptions_isIons	11
GeneralOptions_setIons	
ConfigFile_getIngredients	11
Ingredients_getSize	12
Ingredients_isOmitAtomsER	
Ingredients_getOmitAtomsER	12
Ingredients_setOmitAtomsER	
Ingredients_getComponent	13
Ingredients_addComponent	13
Ingredients_reset	13
ConstructComponent	14
Component_getName	14
Component_setName	15
Component_getMf	15
Component_setMf	15
ConfigFile_getCombustionConditions	15
ConfigFile_getCombustionOptionalConditionsSize	16
ConfigFile_clearCombustionOptionalConditionsList	
ConfigFile_setCombustionOptionalConditions	
ConfigFile_getCombustionOptionalConditions	17
CombustionConditions_getP	17
CombustionConditions_setP	
CombustionConditions_isT	17
CombustionConditions_setT	18
CombustionConditions_getT	18
CombustionConditions_deleteT	
ConfigFile_getHexConditions	19
HEXConditions_getType	
HEXConditions_setType	
HEXConditions_isFreezeOutTemperature	
HEXConditions_getFreezeOutTemperature	
HEXConditions setFreezeOutTemperature	

HEXConditions_isAssignedLoadDensity	21
HEXConditions_setAssignedLoadDensity	21
HEXConditions_getAssignedLoadDensity	21
HEXConditions_getReplaceProductsSize	21
HEXConditions_addReplaceProduct	
HEXConditions_getReplaceProductKey	22
HEXConditions_getReplaceProductValue	
HEXConditions_clearReplaceProducts	
HEXConditions_getIncludeProductsSize	
HEXConditions_addIncludeProduct	23
HEXConditions_getIncludeProduct	24
HEXConditions_clearIncludeProducts	
HEXConditions_getOmitProductsSize	24
HEXConditions_addOmitProduct	25
HEXConditions_getOmitProduct	
HEXConditions_clearOmitProducts	25
Mixture API	26
ConstructMixture	26
DeleteMixture	26
Mixture_size	26
Mixture_add	27
Mixture_add	27
DeleteSpecies	27
Species_getName	28
Species_isReactantOnly	28
Species_isIon	28
Species_getCharge	28
Species_getValence	29
Species_isCondensed	29
Species_getDHf298_15	29
Species_getDH298_15_0	30
Species_getT0	30
Species_getP0	30
Species_getMinimumT	31
Species_getMaximumT	31
Species_getM	31
Species_getR	31
Species_getCp	32
Species_getH	32
Species_getS	32
Species_getG	33
Mixture_getFraction	33
Mixture_setFraction	33
Mixture_checkFractions	
Mixture_getSpecies	
Mixture_getValence	
Mixture_getEquivalenceRatio	35
Mixture_getOxygenBalance	
Mixture_getMolesGas	35
Mixture getM	36

Mixture_getH	
Mixture_getU	36
Mixture_getRho	
Mixture_getFormula	
DeleteFormula	37
Formula_size	37
Formula_getElement	38
Formula_getNumber	38
Equilibrium API	39
ConstructEquilibrium	39
DeleteEquilibrium	39
Equilibrium_setP	39
Equilibrium_setPH	40
Equilibrium_setPT	40
Equilibrium_solve	40
Derivatives_getCp	41
Derivatives_getCv	41
Derivatives_getR	41
Derivatives_getK	42
Derivatives_getGamma	42
Derivatives_getA	42
Derivatives_getRho	43
Derivatives_getRhoGas	43
Derivatives_getZ	43
Derivatives_getM	43
Equilibrium_getP	44
Equilibrium_getT	44
Equilibrium_getH	44
Equilibrium_getU	45
Equilibrium_getS	45
Equilibrium_getG	45
Equilibrium_hasCondensedPhase	46
Equilibrium_getResultingMixture	46
Combustor API	
ConstructCombustor	47
DeleteCombustor	47
Combustor_setP	47
Combustor_setPH	48
Combustor_setPT	48
Combustor_solve	48
Combustor_getEquilibrium	49
Combustor_getDerivatives	49
Combustion Analysis API	50
ConstructCombustionAnalysis	50
DeleteCombustionAnalysis	50
CombustionAnalysis_setPrintResults	
CombustionAnalysis_run	
CombustionAnalysis_isHEX	
CombustionAnalysis_getHEX	
CombustionAnalysis_isHEXInterpolated	

Combustion Analysis g	getCombustorsListSize	.52
5 —	getEquilibrium	
5 —	getDerivatives	

## **Configuration of environment**

To use RPA-C v.2 API for Scilab, the RPA-C dynamic libraries have to be available from the Scilab process. There are two options to achieve that:

- Start Scilab (either GUI or console application) from the installation directory of RPA-C: in Windows command-line console (CMD), go to the installation directory of RPA-C, and start Scilab from there by typing the name of the Scilab executable file an dpressing ENTER
- Add the path to RPA-C installation directory (e.g. "C:\Software\RPA-C") to the environmental variable PATH.

## **Using the API**

To work properly, the Scilab script has to include the following lines in the very beginning:

```
exec loader.sce
RPAInit()
```

Where the file "loader.sce" is a part of RPA-C distribution (you can find it in the root directory of the RPA-C), and "RPAInit()" is am initialization function of the plugin.

When used without parameters (like in two lines above), it will use the paths to thermodynamic libraries, configured in the GUI version of RPA-C (see dialog window Help->Preferences). It can also accept the following string **Parameters:** 

RPAInit(stdThermoPath, stdPropertiesPath, stdTransportPropertiesPath, usrThermoPath, usrPropertiesPath)

## Components

API provides a set of functions to create/get and work with the RPA-C objects.

Most of the functions to work with the RPA-C object accept the reference to the object as a first parameter.

## **Configuration API**

Configuration API is indented for loading, manipulation and writing configuration files. The configuration file can be created in memory and used within RPA-C plugin without saving as a file in a file system of the operating system.

## ConstructConfigFile

Create new configuration object with default values in a memory (no real file is created).

```
ConstructConfigFile()
```

#### **Parameters:**

n.a.

#### Returned value:

Reference to configuration object

#### **Example:**

```
cfg = ConstructConfigFile();
ConfigFile_read(cfg, "test.cfg");
```

## ConfigFile\_read

Read the configuration parameters from the specified file.

```
ConfigFile_read(cfg, path)
```

#### **Parameters:**

cfg Reference to configuration object path File path

#### **Example:**

```
cfg = ConstructConfigFile();
ConfigFile_read(cfg, "test.cfg");
```

## ConfigFile\_write

Write the configuration parameters to the specified file, rewriting the file if already exists.

```
ConfigFile_write(cfg, path)
```

#### **Parameters:**

cfg Reference to configuration object

path File path

```
cfg = ConstructConfigFile();
ConfigFile_write(cfg, "test.cfg");
```

## ConfigFile\_fromString

Read the configuration parameters from the JSON string.

```
ConfigFile_fromString(cfg, json)
```

#### **Parameters:**

cfg Reference to configuration object

json JSON representation of the configuration

#### Example 1:

```
cfg = ConstructConfigFile();
// Use specified JSON string (e.g. from some external file)
ConfigFile_fromString(cfg, "{""HEX_Options"":{""freezeOutTemperature"":
{""unit"":""K"", ""value"":900}, ""type"":""exact
method""}, ""application"":""RPA-C"", ""combustionConditions"":{""pressure"":
{""unit"":"Mpa"", ""value"":20.7}}, ""combustionOptionalConditions"":
[], ""generalOptions"":
{""ions"":false, ""multiphase"":true}, ""info"":""", ""ingredients"":
[], ""name"":""", ""version"":2}");
```

#### **Example 2:**

```
cfg = ConstructConfigFile();
// Prepare Scilab structure with parameters
cfg_struct.application = "RPA-C";
cfg_struct.version = 2;
cfg_struct.name = "test2";
cfg_struct.info = "";
cfg_struct.ingredients = [];
cfg_struct.combustionConditions.pressure.value = 20.7;
cfg_struct.combustionConditions.pressure.unit = "Mpa";
cfg_struct.combustionOptionalConditions = [];
cfg_struct.generalOptions.ions = %F;
cfg_struct.generalOptions.multiphase = %T;
cfg_struct.HEX_Options.type = "exact method";
cfg_struct.HEX_Options.freezeOutTemperature.value = 900;
cfq_struct.HEX_Options.freezeOutTemperature.unit = "K";
// Use Scilab function to JSON to convert structure to JSON string
ison = toJSON(cfg struct);
ConfigFile_fromString(cfg, json);
```

## ConfigFile\_toString

Write the configuration parameters to the JSON string.

```
ConfigFile_toString(cfg)
```

#### Parameters:

cfg Reference to configuration object

#### Returned value:

JSON representation of the configuration

```
cfg = ConstructConfigFile();
ConfigFile_read(cfg, "test.cfg");
json = ConfigFile_toString(cfg);
```

## ConfigFile\_getName

Get the case name.

```
ConfigFile_getName(cfg)
```

#### **Parameters:**

cfg Reference to configuration object

#### Returned value:

Case name

#### **Example:**

```
cfg = ConstructConfigFile();
name = ConfigFile_getName(cfg);
```

## ConfigFile\_setName

Assign the case name.

```
ConfigFile_setName(cfg, name)
```

#### **Parameters:**

cfg Reference to configuration object

name Case name

#### **Example:**

```
cfg = ConstructConfigFile();
ConfigFile_setName(cfg, "Test case");
```

## ConfigFile\_getInfo

Get the case information and comments.

```
ConfigFile_getInfo(cfg)
```

#### **Parameters:**

cfg reference to configuration object

#### Returned value:

Case information and comments

#### **Example:**

```
cfg = ConstructConfigFile();
info = ConfigFile_getInfo(cfg);
```

## ConfigFile\_setInfo

Assign the case information and comments.

```
ConfigFile_setInfo(cfg, info)
```

#### **Parameters:**

cfg Reference to configuration object info Case information and comments

#### **Example:**

```
cfg = ConstructConfigFile();
ConfigFile_setInfo(cfg, "This is a test case comment");
```

## ConfigFile\_getGeneralOptions

Get reference to general options object.

```
ConfigFile_getGeneralOptions(cfg)
```

#### **Parameters:**

cfg Reference to configuration object

#### Returned value:

Reference to general options object

#### **Example:**

```
cfg = ConstructConfigFile();
gopt = ConfigFile_getGeneralOptions(cfg);
```

## GeneralOptions\_isMultiphase

Return %T if multi-phase reaction should be considered.

```
GeneralOptions_isMultiphase(gopt)
```

#### **Parameters:**

gopt Reference to general object

#### Returned value:

Boolean value (%T or %F)

#### **Example:**

```
cfg = ConstructConfigFile();
gopt = ConfigFile_getGeneralOptions(cfg);
m = GeneralOptions_isMultiphase(gopt);
```

## GeneralOptions\_setMultiphase

Set multi-phase flag.

```
GeneralOptions_setMultiphase(gopt, m)
```

#### **Parameters:**

gopt Reference to general object M Boolean value (%T or %F)

```
cfg = ConstructConfigFile();
gopt = ConfigFile_getGeneralOptions(cfg);
GeneralOptions_setMultiphase(gopt, %T);
```

## GeneralOptions\_islons

Return %T if species ionization should be considered.

```
GeneralOptions_isIons(gopt)
```

#### **Parameters:**

gopt Reference to general object

#### Returned value:

Boolean value (%T or %F)

#### **Example:**

```
cfg = ConstructConfigFile();
gopt = ConfigFile_getGeneralOptions(cfg);
m = GeneralOptions_isIons(gopt);
```

## GeneralOptions\_setIons

Set ionization effects flag.

```
GeneralOptions_setIons(gopt, m)
```

#### **Parameters:**

gopt Reference to general object m Boolean value (%T or %F)

#### **Example:**

```
cfg = ConstructConfigFile();
gopt = ConfigFile_getGeneralOptions(cfg);
GeneralOptions_setIons(gopt, %T);
```

## ConfigFile\_getIngredients

Get reference to ingredients list.

```
ConfigFile_getIngredients(cfg)
```

#### **Parameters:**

cfg Reference to configuration object

#### Returned value:

Reference to ingredients list

```
cfg = ConstructConfigFile();
ing = ConfigFile_getIngredients(cfg);
```

## Ingredients\_getSize

Return number of configured ingredients.

```
Ingredients_getSize(ing)
```

#### **Parameters:**

ing Reference to ingredients list

#### Returned value:

Number of configured ingredients

#### **Example:**

```
cfg = ConstructConfigFile();
ing = ConfigFile_getIngredients(cfg);
s = Ingredients_getSize(ing);
```

## Ingredients\_isOmitAtomsER

Return %T (true) if parameter "Omit Atoms from ER calculation" is assigned.

```
Ingredients_isOmitAtomsER(ing)
```

#### **Parameters:**

ing Reference to ingredients list

#### Returned value:

Boolean value (%T or %F)

#### **Example:**

```
cfg = ConstructConfigFile();
ing = ConfigFile_getIngredients(cfg);
if Ingredients_isOmitAtomsER(ing) then
    ...
end
```

## Ingredients\_getOmitAtomsER

Return string with comma-separated list of atoms to omit from ER calculation, or empty string.

```
Ingredients_getOmitAtomsER(ing)
```

#### **Parameters:**

ing Reference to ingredients list

#### Returned value:

String with a comma-separated list of atoms, or empty string

```
cfg = ConstructConfigFile();
ing = ConfigFile_getIngredients(cfg);
atoms = Ingredients_getOmitAtomsER(ing);
```

## Ingredients\_setOmitAtomsER

Assign string with comma-separated list of atoms to omit from ER calculation.

```
Ingredients_setOmitAtomsER(ing, atoms)
```

#### **Parameters:**

ing Reference to ingredients list

atoms String with comma-separated list of atoms, or empty string

#### **Example:**

```
cfg = ConstructConfigFile();
ing = ConfigFile_getIngredients(cfg);
Ingredients_setOmitAtomsER(ing, "Cu,Fe");
```

## Ingredients\_getComponent

Return reference to component specified by index.

```
Ingredients_getComponent(ing, index)
```

#### **Parameters:**

ing Reference to ingredients list index Index of component on teh list

Index 0 corresponds to the first component

#### Returned value:

Reference to component object

#### Example:

```
cfg = ConstructConfigFile();
ing = ConfigFile_getIngredients(cfg);
c = Ingredients_getComponent(ing);
```

## Ingredients\_addComponent

Add new component to the list of ingredients.

```
Ingredients_addComponent(ing, c)
```

#### **Parameters:**

ing Reference to ingredients list c Reference to component object

#### **Example:**

```
cfg = ConstructConfigFile();
ing = ConfigFile_getIngredients(cfg);
c = ConstructComponent("Mg(cr)", 0.1);
Ingredients_addComponent(ing, c);
```

#### Ingredients\_reset

Removes all components from the list of ingredients.

```
Ingredients_reset(ing)
```

#### Parameters:

ing Reference to ingredients list

#### **Example:**

```
cfg = ConstructConfigFile();
ing = ConfigFile_getIngredients(cfg);
Ingredients_reset(ing);
```

#### ConstructComponent

Create component object and return the reference.

```
ConstructComponent(name, massFraction);
```

#### **Parameters:**

name Name of species

Can be empty to create "empty" component (no assigned species)

massFraction Mass fraction of component

Can be empty

Must be empty if name is empty

#### Returned value:

Reference to component object

#### **Example 1:**

```
c1 = ConstructComponent();
c2 = ConstructComponent("Mg(cr)", 0.1);
```

#### **Example 2:**

```
ing = ConfigFile_getIngredients(cfg);
Ingredients_addComponent(ing, ConstructComponent("Si02(qz/crt)", 0.002985));
Ingredients_addComponent(ing, ConstructComponent("AL203(a)", 0.026866));
Ingredients_addComponent(ing, ConstructComponent("GuN03", 0.506294));
Ingredients_addComponent(ing, ConstructComponent("BCN", 0.463855));
```

#### Component\_getName

Return assigned species name.

```
Component_getName(c)
```

#### **Parameters:**

c Reference to component object

#### Returned value:

Assigned name of species

#### **Example:**

```
c = ConstructComponent("Mg(cr)", 0.1);
name = Component_getName(c);
```

#### Component setName

Assign species name.

```
Component_setName(c, name)
```

#### **Parameters:**

c Reference to component object

name Name of species

#### **Example:**

```
c = ConstructComponent();
Component_setName(c, "02(L)");
```

#### Component\_getMf

Return assigned mass fraction.

```
Component_getMf(c)
```

#### **Parameters:**

c Reference to component object

#### Returned value:

Assigned mass fraction

#### **Example:**

```
c = ConstructComponent("Mg(cr)", 0.1);
name = Component_getMf(c);
```

#### Component\_setMf

Assign mass fraction.

```
Component_setMf(c, mf)
```

#### **Parameters:**

c Reference to component object

mf Mass fraction

#### **Example:**

```
c = ConstructComponent();
Component_setName(c, "02(L)");
Component_setMf(c, 0.2);
```

## ConfigFile\_getCombustionConditions

Get reference to main combustion conditions.

```
ConfigFile_getCombustionConditions(cfg)
```

#### Parameters:

cfg Reference to configuration object

#### Returned value:

Reference to main combustion conditions object

```
cfg = ConstructConfigFile();
cc = ConfigFile_getCombustionConditions(cfg);
```

## ConfigFile\_getCombustionOptionalConditionsSize

Return number of configured optional combustion conditions.

ConfigFile\_getCombustionOptionalConditionsSize(cfg)

**Parameters:** 

cfg Reference to configuration object

Returned value:

n.a.

#### **Example:**

s = ConfigFile\_getCombustionOptionalConditionsSize(cfg);

## ConfigFile\_clearCombustionOptionalConditionsList

Remove all configured optional combustion conditions.

ConfigFile\_clearCombustionOptionalConditionsList(cfg)

**Parameters:** 

cfg Reference to configuration object

Returned value:

n.a.

**Example:** 

ConfigFile\_clearCombustionOptionalConditionsList(cfg);

## ConfigFile\_setCombustionOptionalConditions

Add new optional combustion condition.

ConfigFile\_setCombustionOptionalConditions(cfg)

**Parameters:** 

cfg Reference to configuration object

Returned value:

Reference to new optional combustion conditions object

**Example:** 

copt = ConfigFile\_setCombustionOptionalConditions(cfg); // Add new;

## ConfigFile\_getCombustionOptionalConditions

Get optional combustion condition specified by index.

ConfigFile\_getCombustionOptionalConditions(cfg, index)

#### **Parameters:**

cfg Reference to configuration object

Index Index of required optional combustion condition object

#### Returned value:

Reference to optional combustion condition object

#### **Example:**

```
copt = ConfigFile_getCombustionOptionalConditions(cfg, 0);
```

## CombustionConditions\_getP

Get combustion pressure in required units.

CombustionConditions\_getP(c, units)

#### **Parameters:**

c Reference to combustion conditions object

units Required pressure units: "Mpa", "Pa", "bar", "atm", "at", "psi"

#### Returned value:

Pressure in required units

#### **Example:**

```
p = CombustionConditions_getP(c, "Mpa");
```

#### CombustionConditions setP

Set combustion pressure in required units.

CombustionConditions\_setP(c, p, units)

#### **Parameters:**

c Reference to combustion conditions object

p Pressure value

units Required pressure units: "Mpa", "Pa", "bar", "atm", "at", "psi"

#### Returned value:

n.a.

#### **Example:**

```
CombustionConditions_setP(copt, 98.692327, "atm");
```

## CombustionConditions isT

Check whether combustion temperature is specified.

CombustionConditions\_isT(c)

Reference to combustion conditions object

С

#### Returned value:

Boolean value (%F or %T)

#### **Example:**

b = CombustionConditions\_isT(c);

#### CombustionConditions setT

Set required combustion temperature.

CombustionConditions\_setT(c, T, units)

#### **Parameters:**

c Reference to combustion conditions object

T Temperature

units Required temperature units: "K", "C", "R", "F"

#### Returned value:

n.a.

#### **Example:**

CombustionConditions\_setT(c, 1400, "K");

## CombustionConditions\_getT

Return configured combustion temperature.

CombustionConditions\_getT(c, units)

#### Parameters:

c Reference to combustion conditions object

units Required temperature units: "K", "C", "R", "F"

#### Returned value:

Configured combustion temperature in specified units

#### **Example:**

T = CombustionConditions\_getT(c, "K");

#### CombustionConditions\_deleteT

Remove configured combustion temperature.

CombustionConditions\_deleteT(c)

#### **Parameters:**

c Reference to combustion conditions object

#### Returned value:

n.a.

#### **Example:**

CombustionConditions\_deleteT(c);

## ConfigFile\_getHexConditions

Return reference to HEX conditions object.

```
ConfigFile_getHexConditions(cfg)
```

#### **Parameters:**

n.a.

#### Returned value:

Reference to HEX conditions object

#### **Example:**

```
h = ConfigFile_getHexConditions(cfg);
```

## HEXConditions\_getType

Return type of HEX calculation method.

```
HEXConditions_getType(h)
```

#### **Parameters:**

h Reference to HEX conditions object

#### Returned value:

HEX calculation method as a string: "none", "inert diluent method", "exact method"

#### **Example:**

```
type = HEXConditions_getType(h);
```

## HEXConditions\_setType

Set type of HEX calculation method.

```
HEXConditions_setType(h, type);
```

#### **Parameters:**

h Reference to HEX conditions object

type Type of HEX calculation: "none", "inert diluent method", "exact

method"

#### Returned value:

n.a.

```
HEXConditions_setType(h, "exact method");
```

## HEXConditions\_isFreezeOutTemperature

Return %T (true) if freeze-out temperature is specified.

HEXConditions\_isFreezeOutTemperature(h)

#### **Parameters:**

h Reference to HEX conditions object

#### Returned value:

Boolean value (%T or %F)

#### **Example:**

HEXConditions\_isFreezeOutTemperature(h);

## HEXConditions\_getFreezeOutTemperature

Return configured freeze-out temperature in specified units.

HEXConditions\_getFreezeOutTemperature(h, units)

#### **Parameters:**

h Reference to HEX conditions object

units Required temperature units: "K", "C", "R", "F"

#### Returned value:

Freeze-out temperature in specified units

#### Example:

T = HEXConditions\_getFreezeOutTemperature(h, "K");

#### HEXConditions setFreezeOutTemperature

Set freeze-out temperature in specified units.

HEXConditions\_setFreezeOutTemperature(h, T, units)

#### **Parameters:**

h Reference to HEX conditions object

T Temperature value

units Required temperature units: "K", "C", "R", "F"

#### Returned value:

n.a.

#### **Example:**

HEXConditions\_setFreezeOutTemperature(h, 1400, "K");;

## HEXConditions is Assigned Load Density

Return %T (true) if assigned load density is specified.

HEXConditions\_isAssignedLoadDensity(h)

**Parameters:** 

h Reference to HEX conditions object

Returned value:

Boolean value (%T of %F)

**Example:** 

HEXConditions\_isAssignedLoadDensity(h);

## HEXConditions\_setAssignedLoadDensity

Set assigned load density in specified units.

HEXConditions\_setAssignedLoadDensity(h, rho, units)

Parameters:

h Reference to HEX conditions object

rho Load density value

units Required density units: "g/cm^3", "g/cm3", "kg/m^3", "kg/m3"

Returned value:

n.a.

**Example:** 

HEXConditions\_setAssignedLoadDensity(h, 1, "g/cm^3");

## HEXConditions\_getAssignedLoadDensity

Return assigned load density in specified units.

HEXConditions\_getAssignedLoadDensity(h, units)

**Parameters:** 

h Reference to HEX conditions object

units Required density units: "g/cm<sup>3</sup>", "g/cm<sup>3</sup>", "kg/m<sup>3</sup>", "kg/m<sup>3</sup>"

Returned value:

Load density value in specified units

**Example:** 

rho = HEXConditions\_getAssignedLoadDensity(h, "g/cm^3");

## HEXConditions\_getReplaceProductsSize

Return number of replace products.

HEXConditions\_getReplaceProductsSize(h)

Reference to HEX conditions object

#### Returned value:

Number of replace products

#### **Example:**

h

HEXConditions\_getReplaceProductsSize(h);

## HEXConditions\_addReplaceProduct

Add replace product.

HEXConditions\_addReplaceProduct(h, p1, p2)

#### **Parameters:**

h Reference to HEX conditions object

p1 Replaced product name p2 Replacement product name

#### Returned value:

n.a.

#### **Example:**

HEXConditions\_addReplaceProduct(h, "H20", "H20(L)");

## HEXConditions\_getReplaceProductKey

Return the name of replaced product identified by index.

HEXConditions\_getReplaceProductKey(h, index)

#### **Parameters:**

h Reference to HEX conditions object

index Index of replacement paar on the list (starting with 0)

#### Returned value:

Name of replaced product

#### **Example:**

HEXConditions\_getReplaceProductKey(h, 0);

## HEXConditions\_getReplaceProductValue

Return the name of replacement product identified by index.

HEXConditions\_getReplaceProductValue(h, index)

#### **Parameters:**

h Reference to HEX conditions object

index Index of replacement paar on the list (starting with 0)

#### Returned value:

Name of replacement product

#### **Example:**

HEXConditions\_getReplaceProductValue(h, 0);

## HEXConditions\_clearReplaceProducts

Clear the list of replacement products.

HEXConditions\_clearReplaceProducts(h)

**Parameters:** 

h Reference to HEX conditions object

Returned value:

n.a.

#### **Example:**

HEXConditions\_clearReplaceProducts(h);

## HEXConditions\_getIncludeProductsSize

Return number of included products.

HEXConditions\_getIncludeProductsSize(h)

Parameters:

h Reference to HEX conditions object

Returned value:

Number of included products

**Example:** 

HEXConditions\_getIncludeProductsSize(h);

#### HEXConditions\_addIncludeProduct

Add product name to the list of included products.

HEXConditions\_addIncludeProduct(h, p)

**Parameters:** 

h Reference to HEX conditions object

p Product name

**Returned value:** 

n.a.

**Example:** 

HEXConditions\_addIncludeProduct(h, "H20");

## HEXConditions\_getIncludeProduct

Return the included product name specified by index.

HEXConditions\_getIncludeProduct(h, index)

**Parameters:** 

h Reference to HEX conditions object index Product index, starting with 0

Returned value:

Product name

**Example:** 

HEXConditions\_getIncludeProduct(h, 0);

#### HEXConditions clearIncludeProducts

Clear the list of included products.

HEXConditions\_clearIncludeProducts(h)

**Parameters:** 

h Reference to HEX conditions object

Returned value:

n.a.

**Example:** 

HEXConditions\_clearIncludeProducts(h);

## HEXConditions\_getOmitProductsSize

Get number of omitted products.

HEXConditions\_getOmitProductsSize(h)

**Parameters:** 

h Reference to HEX conditions object

Returned value:

Number of omitted products

**Example:** 

HEXConditions\_getOmitProductsSize(h);

#### HEXConditions addOmitProduct

Add product name to the list of omitted products.

HEXConditions\_addOmitProduct(h, p)

#### **Parameters:**

h Reference to HEX conditions object

p Product name

#### Returned value:

n.a.

#### **Example:**

HEXConditions\_addOmitProduct(h, "H20");

## HEXConditions\_getOmitProduct

Get name of omitted product specified by index.

HEXConditions\_getOmitProduct(h, index)

#### **Parameters:**

h Reference to HEX conditions object

index Product index, starting with 0

#### Returned value:

n.a.

#### **Example:**

HEXConditions\_getOmitProduct(h, 0);

## **HEXConditions\_clearOmitProducts**

Clear the list of omitted products.

HEXConditions\_clearOmitProducts(h);

#### **Parameters:**

h Reference to HEX conditions object

#### Returned value:

n.a.

#### **Example:**

HEXConditions\_clearOmitProducts(h);

## **Mixture API**

## ConstructMixture

Construct the mixture object.

```
ConstructMixture()
```

#### **Parameters:**

n.a.

#### Returned value:

Reference to new mixture object

#### **Example:**

```
m = ConstructMixture();
```

#### **DeleteMixture**

Delete the reference to the mixture object.

```
DeleteMixture(m)
```

#### **Parameters:**

m

Reference to mixture object

#### Returned value:

n.a.

#### **Example:**

```
DeleteMixture(m);
```

#### Mixture\_size

Return number of species in the mixture.

```
Mixture_size(m)
```

#### Parameters:

m

Reference to mixture object

#### Returned value:

Number of species in mixture

```
// Gas Yield (mol/kg)
products = Equilibrium_getResultingMixture(e);
v = 1000 / Mixture_getM(products);
v_c = 0;
```

#### Mixture add

Add other mixture to this mixture, assign specified mass fraction, and return reference to species object.

```
s = Mixture_add(m, mix, mf)
```

#### **Parameters:**

m Reference to mixture object

mix Reference to another mixture object

mf Mass fraction of another mixture in this mixture

#### Returned value:

n.a.

#### **Example:**

```
Mixture_add(m, mix, 0.3);
```

#### Mixture add

Add species to the mixture, assign specified mass fraction, and return reference to species object.

```
s = Mixture_add(m, name, mf)
```

#### Parameters:

m Reference to mixture object

name Species name

mf Mass fraction of species in the mixture

#### Returned value:

Reference to the species object added to the mixture

#### **Example:**

```
s = Mixture\_add(m, "H2O(L)", 1.0);
```

#### **DeleteSpecies**

Delete the reference to the species object.

```
DeleteSpecies(s)
```

#### Parameters:

s Reference to the species object

#### Returned value:

n.a.

#### **Example:**

DeleteSpecies(s);

## Species\_getName

Return species name.

```
Species_getName(s)
```

#### **Parameters:**

S

Reference to the species object

#### Returned value:

Species name

#### **Example:**

```
name = Species_getName(s);
```

#### Species\_isReactantOnly

Return %T (true) if species could not be usually used as a propellant component.

```
Species_isReactantOnly(s)
```

#### **Parameters:**

s

Reference to the species object

#### Returned value:

Boolean value

#### **Example:**

Species\_isReactantOnly(s);

## Species\_islon

Return %T (true) if species is ionized.

```
Species_isIon(s)
```

#### **Parameters:**

S

Reference to the species object

#### Returned value:

Boolean value

#### **Example:**

```
Species_isIon(s);
```

## Species\_getCharge

Return the charge of ionized species.

```
Species_getCharge(s)
```

**Parameters:** 

s Reference to the species object

Returned value:

Charge of species

**Example:** 

```
c = Species_getCharge(s);
```

#### Species\_getValence

Return the valency of species.

```
Species_getValence(s)
```

**Parameters:** 

s Reference to the species object

Returned value:

Valency of species

Example:

```
v = Species_getValence(s);
```

#### Species\_isCondensed

Return %T (true) if species is condensed.

Species\_isCondensed(s)

Parameters:

s Reference to the species object

Returned value:

Boolean value

Example:

Species\_isCondensed(s);

#### Species\_getDHf298\_15

Return  $H^0(298.15)$  - heat of formation at the temperature 298.15 K and pressure 1 bar in desired units.

```
Species_getDHf298_15(s, units)
```

Parameters:

s Reference to the species object

units Result units: "J/mol", "J/kg", "kJ/kg"

Returned value:

Heat of formation

#### **Example:**

```
hf = Species_getDHf298_15(s, "J/mol");
```

## Species getDH298\_15\_0

Return  $H^0(298.15) - H^0(0)$  in desired units, if available.

```
Species_getDH298_15_0(s, units)
```

#### **Parameters:**

s Reference to the species object

units Result units: "J/mol", "J/kg", "kJ/kg"

#### Returned value:

```
H^{0}(298.15) - H^{0}(0)
```

#### **Example:**

```
dh = Species\_getDH298\_15\_0(s, "J/mol");
```

#### Species\_getT0

Return standard temperature of the species in desired units.

```
Species_getT0(s, units)
```

#### **Parameters:**

s Reference to the species object

units Temperature units: "K", "C", "R", "F"

#### Returned value:

Standard temperature

#### **Example:**

```
T0 = Species_getT0(s, "K");
```

#### Species getP0

Return standard pressure of the species in desired units.

```
Species_getP0(s, units)
```

#### Parameters:

s Reference to the species object

units Pressure units: "Mpa", "Pa", "bar", "atm", "at", "psi"

#### Returned value:

Standard pressure

```
p0 = Species_getP0(s, "Pa");
```

#### Species\_getMinimumT

Return minimum temperature of the species in desired unit.

```
Species_getMinimumT(s, units)
```

#### **Parameters:**

s Reference to the species object

units Temperature units: "K", "C", "R", "F"

#### Returned value:

Minimum temperature

#### **Example:**

```
Tmin = Species_getMinimumT(s, "K");
```

## Species\_getMaximumT

Return maximum temperature of the species in desired unit.

```
Species_getMaximumT(s, units)
```

#### **Parameters:**

s Reference to the species object

units Temperature units: "K", "C", "R", "F"

#### Returned value:

Maximum temperature

#### **Example:**

```
Tmax = Species_getMaximumT(s, "K");
```

#### Species getM

Return molecular weight of species.

```
Species_getM(s)
```

#### Parameters:

s Reference to the species object

#### **Returned value:**

Molecular weight of species

#### **Example:**

```
M = Species_getM(s);
```

## Species\_getR

Get gas constant in desired unit (applicable for gaseous species only).

```
Species_getR(s, units)
```

s Reference to the species object

units Gas constant units: "J/(mol K)", "J/(kg K)", "kJ/(kg K)"

#### Returned value:

Gas constant in desired unit

#### **Example:**

```
R = Species_getR(s, "J/(mol K)");
```

#### Species\_getCp

Return specific heat or molar heat capacity (depending on desired units) at specified temperature and constant pressure in desired units.

```
Species_getCp(s, T, tunits, runits)
```

#### **Parameters:**

s Reference to the species object

T Temperature value

tunits Temperature units: "K", "C", "R", "F"

runits Result units: "J/(mol K)", "J/(kg K)", "kJ/(kg K)"

#### Returned value:

Specific heat or molar heat capacity (depending on desired units)

#### **Example:**

```
cp = Species_getCp(s, 1300, "J/(kg K)");
```

## Species\_getH

Return specific or molar enthalpy (depending on desired units) at specified temperature in desired units.

```
Species_getH(s, T, tunits, runits)
```

#### **Parameters:**

s Reference to the species object

T Temperature value

tunits Temperature units: "K", "C", "R", "F" runits Result units: "J/mol", "J/kg", "kJ/kg"

#### Returned value:

Specific or molar enthalpy

#### **Example:**

```
h = Species_getH(s1, 1300, "K", "J/mol");
```

#### Species\_getS

Return specific or molar entropy (depending on desired units) at specified temperature in desired units.

```
Species_getS(s, T, tunits, runits)
```

s Reference to the species object

T Temperature value

tunits Temperature units: "K", "C", "R", "F"

runits Result units: "J/(mol K)", "J/(kg K)", "kJ/(kg K)"

#### Returned value:

Specific or molar entropy

#### **Example:**

```
s = Species_getS(s, 1300, "K", "J/(mol K)");
```

#### Species\_getG

Get Gibbs energy of species at specified temperature.

```
Species_getG(s, T, tunits, runits)
```

#### Parameters:

s Reference to the species object

T Temperature value

tunits Temperature units: "K", "C", "R", "F" runits Result units: "J/mol", "J/kg", "kJ/kg"

#### Returned value:

Gibbs energy of species at specified temperature

#### **Example:**

```
g = Species_getG(s, 1300, "K", "J/mol");
```

## Mixture getFraction

Return mass fraction assigned to the species identified by given index.

```
Mixture_getFraction(m, index)
```

## Parameters:

m Reference to mixture object

index Species index

#### Returned value:

Mass fraction

#### **Example:**

```
mf = Mixture_getFraction(m, 0);
```

#### Mixture setFraction

Assign mass fraction to the species identified by given index.

```
Mixture_setFraction(m, index, mf)
```

m Reference to mixture object

index Species index

#### Returned value:

n.a.

#### **Example:**

```
Mixture_setFraction(m, 0, 0.7);
```

#### Mixture checkFractions

Return %T (true) if mass fractions assigned correctly (that is, the sum of all mass fractions is equals to 1.0). If parameter

```
Mixture_checkFractions(m, fix)
```

#### **Parameters:**

m Reference to mixture object

fix If %T (true), the mass fractions will be re-assigned automatically to get teh sum=1.0

#### Returned value:

Boolean value

#### **Example:**

```
Mixture_checkFractions(m, %T);
```

## Mixture\_getSpecies

Return reference to species object identified by given index.

```
Mixture_getSpecies(m, index)
```

#### Parameters:

m Reference to mixture object index Species index, starting with 0

#### Returned value:

n.a.

#### **Example:**

```
s = Mixture_getSpecies(m, 0);
```

## Mixture\_getValence

Get total mixture valency.

```
Mixture_getValence(m)
```

#### **Parameters:**

m Reference to mixture object

#### Returned value:

Mixture valency

#### Example:

```
v = Mixture_getValence(m);
```

## Mixture\_getEquivalenceRatio

Get mixture equivalence ratio.

```
Mixture_getEquivalenceRatio(m)
```

**Parameters:** 

m Reference to mixture object

Returned value:

Equivalence ratio

Example:

```
eq = Mixture_getEquivalenceRatio(m);
```

## Mixture\_getOxygenBalance

Get mixture oxygen balance.

```
Mixture_getOxygenBalance(m)
```

**Parameters:** 

m Reference to mixture object

Returned value:

Oxygen balance

**Example:** 

```
ob = Mixture_getOxygenBalance(m);
```

## Mixture\_getMolesGas

Get moles of gas in mixture in desired units.

```
Mixture_getMolesGas(m, units)
```

**Parameters:** 

m Reference to mixture object

units Result units: "mol/kg", "mol/g", "mol/100g"

Returned value:

Moles of gas

```
// Get the density of the initial mixture
rho = Mixture_getRho(mix, "kg/m^3");
```

```
T = Equilibrium_getT(e, "K");
products = Equilibrium_getResultingMixture(e);
g = Mixture_getMolesGas(products, "mol/kg");  // mol/kg
volGasYield = rho * g / 10000;  // mol/100cm³
MSIFx = T * g / 1000;  // mol·K/g
```

## Mixture\_getM

Get molecular weight of mixture.

```
Mixture_getM(m)
```

#### **Parameters:**

m Reference to mixture object

#### Returned value:

Molecular weight

#### **Example:**

```
M = Mixture_getM(m);
```

## Mixture\_getH

Get specific or molar enthalpy of mixture in desired units.

```
Mixture_getH(m, units)
```

#### **Parameters:**

m Reference to mixture object

units Result units: "J/mol", "J/kg", "kJ/kg"

#### Returned value:

Specific or molar enthalpy of mixture

#### **Example:**

```
h = Mixture_getH(m, "J/mol");
```

#### Mixture\_getU

Get specific or molar internal energy of mixture in desired units.

```
Mixture_getU(m, units)
```

#### **Parameters:**

m Reference to mixture object

units Result units: "J/mol", "J/kg", "kJ/kg"

#### **Returned value:**

Specific or molar internal energy of mixture

```
u = Mixture_getU(m, "J/mol");
```

# Mixture\_getRho

Get density of mixture in desired units.

```
Mixture_getRho(m, units)
```

#### **Parameters:**

m Reference to mixture object

units Result units: "g/cm<sup>3</sup>", "g/cm<sup>3</sup>", "kg/m<sup>3</sup>", "kg/m<sup>3</sup>"

#### Returned value:

Density of mixture

### **Example:**

```
rho = Mixture_getRho(m, "kg/m^3");
```

# Mixture getFormula

Get reference to exploded formula object.

```
Mixture_getFormula(m, basedOn)
```

### **Parameters:**

m Reference to mixture object

basedOn Type of exploded formula: "%", "kg", "g"

#### Returned value:

Reference to exploded formula object

### **Example:**

```
f = Mixture_getFormula(m, "%");
```

## **DeleteFormula**

Delete reference to exploded formula object.

```
DeleteFormula(f);
```

#### **Parameters:**

f Reference to exploded formula object

#### Returned value:

n.a.

#### **Example:**

```
DeleteFormula(f);
```

## Formula size

Number of chemical elements in exploded formula.

```
Formula_size(f)
```

#### **Parameters:**

f Reference to exploded formula object

#### Returned value:

Number of chemical elements

#### **Example:**

```
n = Formula_size(f);
```

# Formula\_getElement

Get name of chemical element identified by index.

```
Formula_getElement(f, index)
```

### **Parameters:**

f Reference to exploded formula object

index Index of chemical element in exploded formula, starting with 0

#### Returned value:

Name of chemical element

## **Example:**

```
name = Formula_getElement(f, 0);
```

# Formula\_getNumber

Get amount of chemical element in exploded formula.

```
Formula_getNumber(f, index)
```

#### **Parameters:**

f Reference to exploded formula object

index Index of chemical element in exploded formula, starting with 0

## Returned value:

Amount of chemical element

```
n = Formula getNumber(f, 0);
```

# **Equilibrium API**

# ConstructEquilibrium

Create equilibrium object based on provided mixture of ingredients.

```
ConstructEquilibrium(m)
```

Parameters:

m Reference to mixture object

### Returned value:

Reference to equilibrium object

### **Example:**

```
e = ConstructEquilibrium(m);
```

# DeleteEquilibrium

Delete equilibrium object.

```
DeleteEquilibrium(e)
```

### **Parameters:**

e Reference to equilibrium object

#### Returned value:

n.a.

## **Example:**

```
DeleteEquilibrium(e);
```

# Equilibrium\_setP

Assign combustion pressure, switching the solving reaction problem to type (p,H)=const. Enthalpy of mixture of ingredients is automatically calculated using mixture assigned in constructor.

```
Equilibrium_setP(e, p, punits)
```

## Parameters:

e Reference to equilibrium object

p Pressure value

punits Pressure units: "Mpa", "Pa", "bar", "atm", "at", "psi"

### Returned value:

n.a.

```
Equilibrium_setP(e, 20, "MPa");
```

# Equilibrium\_setPH

Assign combustion pressure and specified enthalpy, switching reaction problem to type (p,H)=const.

```
Equilibrium_setPH(e, p, punits, H, hunits)
```

#### **Parameters:**

e Reference to equilibrium object

p Pressure value

punits Pressure units: "Mpa", "Pa", "bar", "atm", "at", "psi"

H Enthalpy value

hunits Enthalpy units: "J/mol", "kJ/mol"

#### Returned value:

n.a.

#### **Example:**

```
Equilibrium_setPH(e, 20, "MPa", Mixture_getH(m, "J/mol"), "J/mol");
```

# Equilibrium setPT

Assign pressure and temperature of combustion, switching reaction problem to type (p,T)=const.

```
Equilibrium_setPT(e, p, punits, T, tunits)
```

#### **Parameters:**

e Reference to equilibrium object

p Pressure value

punits Pressure units: "Mpa", "Pa", "bar", "atm", "at", "psi"

T Temperature value

tunits Temperature units: "K", "C", "R", "F"

#### Returned value:

n.a.

## **Example:**

```
Equilibrium_setPT(e, 20, "MPa", 1274.6012, "K");
```

# Equilibrium\_solve

Solve the configured equilibrium problem and get the reference to derivatives object.

In some cases the problem does not converge because condensed species not included before first iteration. To solve such a problems, set parameter z to true.

```
Equilibrium_solve(e, z)
```

#### **Parameters:**

e Reference to equilibrium object

z If %T (true) include condensed species into the reaction

Optional parameter; defailt value is %T

### Returned value:

Reference to derivatives object

## **Example:**

```
d = Equilibrium_solve(e);
d = Equilibrium_solve(e, %F);
```

# Derivatives\_getCp

Get specific heat or molar heat capacity of reaction products at constant pressure in desired units.

```
Derivatives_getCp(d, units)
```

#### **Parameters:**

d Reference to derivatives object

units Result units: "J/(kg K)", "kJ/(kg K)", J/(mol K)

#### Returned value:

Specific heat or molar heat capacity Cp

#### **Example:**

```
Cp = Derivatives_getCp(d, "J/(mol K)");
```

# Derivatives\_getCv

Get specific heat or molar heat capacity of reaction products at constant volume in desired units.

```
Derivatives_getCv(d, units)
```

#### **Parameters:**

d Reference to derivatives object

units Result units: "J/(kg K)", "kJ/(kg K)", J/(mol K)

#### Returned value:

Specific heat or molar heat capacity Cv

## **Example:**

```
Cv = Derivatives_getCv(d, "J/(mol K)");
```

## Derivatives getR

Get gas constant of reaction products in desired units.

```
Derivatives_getR(d, units)
```

#### **Parameters:**

d Reference to derivatives object

units Result units: "J/(kg K)", "kJ/(kg K)", J/(mol K)

#### Returned value:

Gas constant R

## **Example:**

```
R = Derivatives_getR(d, "J/(mol K)");
```

# Derivatives\_getK

Get isentropic exponent of reaction products.

```
Derivatives_getK(d)
```

### **Parameters:**

d Reference to derivatives object

### Returned value:

Isentropic exponent

### **Example:**

```
k = Derivatives_getK(d);
```

# Derivatives\_getGamma

Get specific heat ratio of reaction products.

```
Derivatives_getGamma(d)
```

#### **Parameters:**

d Reference to derivatives object

#### Returned value:

Specific heat ratio of reaction products

### **Example:**

```
gamma = Derivatives_getGamma(d);
```

# Derivatives\_getA

Get velocity of sound in desired units.

```
Derivatives_getA(d, units)
```

#### **Parameters:**

d Reference to derivatives object

units Result units: "m/s"

#### Returned value:

Velocity of sound

```
a = Derivatives_getA(d, "m/s");
```

# Derivatives\_getRho

Get density of reaction products in desired units.

```
Derivatives_getRho(d, units)
```

#### **Parameters:**

d Reference to derivatives object units Result units: "kg/m^3", "g/m^3"

#### Returned value:

Density of reaction products

### **Example:**

```
rho = Derivatives_getRho(d, "kg/m^3");
```

# Derivatives\_getRhoGas

Get density of gaseous reaction products in desired units.

```
Derivatives_getRhoGas(d, units)
```

#### **Parameters:**

d Reference to derivatives object units Result units: "kg/m^3", "g/m^3"

#### Returned value:

Density of gaseous reaction products

### **Example:**

```
rho_gas = Derivatives_getRhoGas(d, "kg/m^3");
```

# Derivatives\_getZ

Get mass fraction of condensed reaction products.

```
Derivatives_getZ(d)
```

### **Parameters:**

d Reference to derivatives object

#### Returned value:

Mass fraction of condensed reaction products

### **Example:**

```
z = Derivatives_getZ(d);
```

# Derivatives\_getM

Get molecular weight of reaction products.

```
Derivatives_getM(d)
```

Parameters:

d Reference to derivatives object

#### Returned value:

Molecular weight of reaction products

#### **Example:**

```
M = Derivatives_getM(d);
```

# Equilibrium\_getP

Get assigned pressure of reaction.

```
Equilibrium_getP(e, units)
```

### **Parameters:**

e Reference to equlibrium object

units Pressure units: "Mpa", "Pa", "bar", "atm", "at", "psi"

#### Returned value:

Pressure of reaction

## **Example:**

```
p = Equilibrium_getP(e, "MPa");
```

# Equilibrium\_getT

Get the temperature of reaction.

```
Equilibrium_getT(e, units)
```

### **Parameters:**

e Reference to equlibrium object

units Temperature units: "K", "C", "R", "F"

## Returned value:

Temperature of reaction

#### **Example:**

```
T = Equilibrium_getT(e, "K");
```

# Equilibrium\_getH

Get specific or molar enthalpy of reaction products.

```
Equilibrium_getH(e, units)
```

### **Parameters:**

e Reference to equlibrium object

units Enthalpy units: "J/mol", "kJ/mol", "J/kg", "kJ/kg"

#### Returned value:

Enthalpy of reaction products

### **Example:**

```
H = Equilibrium_getH(e, "J/mol");
```

# Equilibrium getU

Get specific or molar internal energy of reaction products.

```
Equilibrium_getU(e, units)
```

#### **Parameters:**

e Reference to equlibrium object

units Internal energy units: "J/mol", "kJ/mol", "J/kg", "kJ/kg"

#### Returned value:

Internal energy of reaction products

### **Example:**

```
U = Equilibrium_getU(e, "J/mol");
```

# Equilibrium\_getS

Get specific or molar entropy of reaction products.

```
Equilibrium_getS(e, units)
```

## **Parameters:**

e Reference to equlibrium object

units Entropy units: "J/(mol K)", "J/(kg K)", "kJ/(kg K)"

# Returned value:

Entropy of reaction products

#### **Example:**

```
S = Equilibrium_getS(e, "J/(mol K)");
```

# Equilibrium\_getG

Get Gibbs energy of reaction products.

```
Equilibrium_getG(e, units)
```

### Parameters:

e Reference to equlibrium object

units Gibbs energy units: "J/mol", "kJ/mol", "J/kg", "kJ/kg"

#### Returned value:

Gibbs energy of reaction products

# Example:

```
G = Equilibrium_getG(e, "J/mol");
```

# Equilibrium\_hasCondensedPhase

Get %T (true) if reaction products contains condensed species.

Equilibrium\_hasCondensedPhase(e)

### **Parameters:**

е

Reference to equlibrium object

## **Returned value:**

Boolean value (%T or %F)

### Example:

Equilibrium\_hasCondensedPhase(e);

# Equilibrium\_getResultingMixture

Get reference to Mixture object, containing all products of reaction.

Equilibrium\_getResultingMixture(e)

#### **Parameters:**

е

Reference to equlibrium object

### Returned value:

Reference to Mixture object

```
rm = Equilibrium_getResultingMixture(e);
```

# **Combustor API**

## ConstructCombustor

Create Combustor object using given object Mixture with ingrediants.

ConstructCombustor(m)

## Parameters:

m

Reference to mixture object

### Returned value:

Reference to Combustor object

### **Example:**

```
c = ConstructCombustor(m);
```

## **DeleteCombustor**

Delete combustor object.

```
DeleteCombustor(c);
```

#### **Parameters:**

С

Reference to combustor object

#### Returned value:

n.a.

### **Example:**

DeleteCombustor(c);

## Combustor\_setP

Assign combustion chamber pressure, switching the solving reaction problem to type (p,H)=const.. Enthalpy of mixture of ingredients is automatically calculated using mixture assigned in constructor.

```
Combustor_setP(c, p, punits)
```

#### **Parameters:**

c Reference to combustor object

p Pressure value

punits Pressure units: "Mpa", "Pa", "bar", "atm", "at", "psi"

#### Returned value:

n.a.

```
Combustor_setP(c, 20, "Mpa");
```

# Combustor setPH

Assign combustion pressure and specified enthalpy, switching reaction problem to type (p,H)=const.

```
Combustor_setPH(c, p, punits, H, hunits)
```

#### **Parameters:**

c Reference to combustor object

p Pressure value

punits Pressure units: "Mpa", "Pa", "bar", "atm", "at", "psi"

H Enthalpy value

hunits Enthalpy units: "J/mol", "kJ/mol"

#### Returned value:

n.a.

#### **Example:**

```
Combustor_setPH(c, 20, "MPa", Mixture_getH(m, "J/mol"), "J/mol");
```

# Combustor setPT

Assign pressure and temperature of combustion, switching reaction problem to type (p,T)=const.

```
Combustor_setPT(c, p, punits, T, tunits)
```

#### **Parameters:**

c Reference to combustor object

p Pressure value

punits Pressure units: "Mpa", "Pa", "bar", "atm", "at", "psi"

T Temperature value

tunits Temperature units: "K", "C", "R", "F"

## Returned value:

n.a.

### **Example:**

```
Combustor_setPT(c, 20, "MPa", 1274.6012, "K");
```

## Combustor solve

Solve the chemical equilibrium problem.

In some cases the problem does not converge because condensed species not included before first iteration. To solve such a problems, set parameter z to true.

```
Combustor_solve(c, z)
```

#### **Parameters:**

c Reference to combustor object

z If %T (true) include condensed species into the reaction

Optional parameter; defailt value is %T

#### Returned value:

n.a.

## **Example:**

```
Combustor_solve(c);
Combustor_solve(c, %T)
```

# Combustor\_getEquilibrium

Get reference to object Equilibrium for solved chemical equilibrium problem.

```
Combustor_getEquilibrium(c)
```

#### **Parameters:**

С

Reference to combustor object

## Returned value:

Reference to equilibrium object

## **Example:**

```
e = Combustor_getEquilibrium(c);
```

# Combustor\_getDerivatives

Get regerence to object Derivatives for solved chemical equilibrium problem.

```
Combustor_getDerivatives(c)
```

### **Parameters:**

С

Reference to combustor object

### **Returned value:**

Reference to derivatives object

```
d = Combustor_getDerivatives(c);
```

# **Combustion Analysis API**

# ConstructCombustionAnalysis

Create combustion analysis object.

ConstructCombustionAnalysis()

#### **Parameters:**

n.a.

### Returned value:

Reference to combustion analysis object

### **Example:**

```
ca = ConstructCombustionAnalysis();
```

# **DeleteCombustionAnalysis**

Delete combustion analysis object.

DeleteCombustionAnalysis(ca)

### **Parameters:**

ca Reference to combustion analysis object.

#### Returned value:

n.a.

## **Example:**

DeleteCombustionAnalysis(ca);

# CombustionAnalysis\_setPrintResults

Configure the verbose logging mode.

```
CombustionAnalysis_setPrintResults(ca, print);
```

#### **Parameters:**

ca Reference to combustion analysis object

print If %T (true), set the verbose logging mode while running the analysis

## Returned value:

n.a.

```
ca = ConstructCombustionAnalysis();
CombustionAnalysis_setPrintResults(ca, %F);
CombustionAnalysis_run(ca, cfg);
```

# CombustionAnalysis\_run

Execute the problem configured in given configuration file.

```
CombustionAnalysis_run(ca, cfg);
```

#### **Parameters:**

ca Reference to combustion analysis object.

cfg Reference to configuration object.

#### Returned value:

n.a.

### **Example:**

```
cfg = ConstructConfigFile();
ConfigFile_read(cfg, "test.cfg");
ca = ConstructCombustionAnalysis();
CombustionAnalysis_run(ca, cfg);
```

# CombustionAnalysis\_isHEX

Return %T (true) if HEX was configured and calculated.

```
CombustionAnalysis_isHEX(ca)
```

#### **Parameters:**

ca Reference to combustion analysis object.

#### Returned value:

Boolean value (%T or %F)

#### **Example:**

CombustionAnalysis\_isHEX(ca);

# CombustionAnalysis\_getHEX

Get calculated HEX in specified unts.

```
CombustionAnalysis_getHEX(ca, units)
```

### **Parameters:**

```
ca Reference to combustion analysis object.
```

units Result units: "J/kg", "kJ/kg", "kcal/kg", "Btu/lbm"

### Returned value:

n.a.

```
hex = CombustionAnalysis_getHEX(ca, "J/kg");
```

# CombustionAnalysis\_isHEXInterpolated

Return %T (true) if HEX was interpolated.

CombustionAnalysis\_isHEXInterpolated(ca)

**Parameters:** 

ca Reference to combustion analysis object.

Returned value:

Boolean %T if HEX is interpolated

**Example:** 

CombustionAnalysis\_isHEXInterpolated(ca);

# CombustionAnalysis\_getCombustorsListSize

Return number of combustors, including the combustor for the main combustion conditions as well as all combustors for optional combustion condistions.

CombustionAnalysis\_getCombustorsListSize(ca)

**Parameters:** 

ca Reference to combustion analysis object.

Returned value:

Number of available combustors

**Example:** 

size = CombustionAnalysis\_getCombustorsListSize(ca);

# CombustionAnalysis\_getEquilibrium

Return reference to equilibrium object for specified index.

CombustionAnalysis\_getEquilibrium(ca, index);

**Parameters:** 

ca Reference to combustion analysis object.

index Combustion condition index.

Index 0 corresponds to main combustion conditions. Index > 0 corresponds to optional combustion conditions.

Returned value:

Reference to equilibrium object

# CombustionAnalysis\_getDerivatives

Return reference to derivatives object for specified index.

```
CombustionAnalysis_getDerivatives(ca, index);
```

### **Parameters:**

ca Reference to combustion analysis object.

index Combustion condition index.

Index 0 corresponds to main combustion conditions. Index > 0 corresponds to optional combustion conditions.

#### Returned value:

Reference to derivatives object