PROPOSAL for addition of Chemical Species in SIDS −
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GasModel_t Data Structure

The GasModel_t data structure will be defined as follow in the SIDS:
GasModelType_t is an enumeration type that describes the type of gas model:

```
  GasModelType_t := Enumeration(
    Null,
    Ideal,
    FiniteRate
    Equilibrium,
    Frozen,
    LiuVinokur,
    Tannehill ) ;

GasModel_t :=
  {
  List( Descriptor_t Descriptor1 ... DescriptorN ) ;       (o)
  GasModelType_t GasModelType ;                            (r)
  ThermodynamicsModelType_t ThermodynamicsModelType ;      (o)
  List( DataArray_t<DataType, 1, 1> DataArray1 ...
                                    DataArrayN ) ;         (o)
  }
```

The proposal adds new types of gas model to GasModelType_t. It also eliminates VanderWaals as a GasModelType_t type and creates an optional Descriptor_t called ThermodynamicsModel_t.

The GasModelTypes can be briefly described as:

- Ideal − The ideal gas equations can be used, constant specific heats, P=rho*R*T.
- FiniteRate − Finite rate chemical reactions are taking place. There are reaction equations for various species. Reactants take finite time to react.
- Equilibrium − Implies chemical reactions are infinitely fast relative to the residence time of the mixture in a cell. Thus all reactions go to completion. Equilibrium here implies that species are being tracked and equations take place, but reaction rates are infinite.
- Frozen − Assumes that chemical reactions are infinitely slow. Species may be specified and mix, but no reactions take place.
- LiuVinokur, Tannehill − The tables of Liu and Vinokur, or Tannehill are used to evaluate the properties of equilibrium air at various temperatures and pressures. That is, no species or equations are tracked, the thermodynamic properties are found via table lookup.

ThermodynamicsModelType describes the thermodynamics model used and has the following pre−defined values:

```
ThermodynamicsModelType_t := Enumeration (
  Null,
  CaloricallyPerfect,
  ThermallyPerfect,
  VanderWaals ) ;
```

If ThermodynamicsModel_t is not present the thermodynamics model will default to ThermallyPerfect except in the case of ideal, where CaloricallyPerfect is assumed.

For reference, CaloricallyPerfect implies that the specific heats are constant and ThermallyPerfect that they are functions of temperature only. Other models define other approximations for the specific heats that become functions of temperature and pressure.

There may be other GasModelTypes and ThermodynamicModelTypes in use. The list is based on current CFD implementations. Users are encouraged to send additional model names, and a brief description to extend the list.

Currently, CGNS does not have a way to store the functional form of the variation of the chemistry properties, reactions and rates, equilibrium tables, or transport properties. It is up to the application to interpret the model used, and provide appropriate functionality. The definition of these functional forms may be the subject of a future extension.

It is also proposed to add the following data−name identifiers for the DataArray_t nodes recorded in the GasModel_t data structure:

- MolecularWeight*Symbol*
- HeatOfFormation*Symbol*
- FuelAirRatio

The variable *Symbol* in the data−name identifiers should be replaced with the chemical symbol of the species. The table on the right proposes a preliminary list of symbols. It is proposed that any chemical symbol can be used, the table lists examples only. In addition, mixtures can be defined by conventional names. However, additional mixture names should be proposed as SIDS extensions to ensure consistency. As always, individual users can define new names, and in this case *symbol*, but these names may not be recognized by other CGNS compliant applications unless registered.

Symbol	**Specie**
PHI	Fuel air ratio
H	Hydrogen
N	Nitrogen
O	Oxygen
H2	Hydrogen Molecule
N2	Nitrogen Molecule
O2	Oxygen Molecule
OH	Hydroxide
NO	Nitric Oxide
N2O	Nitrous Oxide
NO2	Nitrogen dioxide
H2O	Water
CN	
CNO	
CNO+	
CN2	
CO	Carbon monoxide
CO2	Carbon dioxide
NO+	
HO2	
H2O2	
RP1	
JP5	Jet fuel
JP7	Jet fuel
JP10	Jet fuel
e−	Electrons

ViscosityModelType_t

ViscosityModelType_t is an enumeration type that describes the type of viscosity model:

```
ViscosityModelType_t := Enumeration(
  Null,
  Constant,
  PowerLaw,
  SutherlandLaw,
  WilkesLaw,
  KeysLaw ) ;
```

Constant, PowerLaw and SutherlanLaw potentially have data associated with them that may be stored as DataArrays under the ViscosityModelType_t. (See current SIDS).

WilkesLaw and KeysLaw use the transport properties of each species of a mixture to compute the effective viscosity. We do not attempt to store the species properties in the CGNS file at present, it is up to the application to provide the required functionality. Means of storing this data may be the subject of a future extension.

There may be other common means of predicting the transport properties. Users are encouraged to submit proposed names, descriptions, and potentially new data name identifiers to extend this list.

New data−name identifiers for solution data

The primary requirement to support chemical information is to add additional data−name identifiers to record the chemical state. It is proposed that the following data−name identifiers be added to the SIDS. These should serve to record field data under the FlowSolution_t nodes.

Data−Name Identifier	Description	Units
MassFractionSymbol	Mass fraction of species defined by Symbol	M/M
LaminarViscositySymbol	Laminar viscosity of the species defined by Symbol	M/(LT)
ThermalConductivitySymbol		$ML/(T^3\Theta)$
BinaryDiffusionCoefficientSymbol		L^2/T
EffectiveSpecificHeatRatio	Beta=h/e (of mixture) Used in energy equation. Integrated from stagnation conditions, path dependant. Note: the local SpecificHeatRatio is already defined	−
CompressibilityFactor	Z=R/Rinf = Gas constant of the mixture / Freestream gas constant	−
VibrationalElectronEnergy	Vibrational−electronic excitation energy per unit volume	L^2/T^2
HeatOfFormation	Summation of the heat of formation of all species	L^2/T^2
VibrationalElectronTemperature	Vibrational electron temperature	Θ

Notes:

- There are obviously many chemical species of potential interest (such as hydrocarbon species). It is proposed to define MassFraction*Symbol* where *Symbol* is the common chemical symbol for the species.

- Users who need additional species are encouraged to send the definition of these species to the CGNS team so they can be added to the SIDS.

CGNS Library Extension:

- At present it is not proposed to define mole fraction, partial density, or molar concentration information in the SIDS. However, we realize that these may also be of interest, and may be added in the future. Since there is are unique 1−1 mappings of mass fraction to these other quantities, we recommend building in conversions between them in the mid−level libraries, so users can store or request either, with the mid−level libraries doing the proper conversion.

Open issue:

- At this point, we have no way of defining the reaction rate equations, or the curve fits of enthalpy as a function of the temperature for various species. This will not be

addressed under this extension. The application must supply the information in whatever form is required. The defninition of this information could be covered by a future extension. Questions to be addressed include: Would we need buy−in from chemistry codes, which create the data? Would the definition of such information under the SIDS imply a level of utilities we want to support (curve fit routines, etc.)?