

Proposal for addition of Chemical Species in the SIDS –
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The ElementalComposition_t data structure will be defined as follows in the SIDS:

```
ElementalComposition_t :=  
{  
List(float StoichiometricCoeff1 ... StoichiometricCoeffNumberElements);  
}
```

The RangeModel_t data structure will be defined as follows in the SIDS:

```
RangeModel_t :=  
{  
float[7] JanafPolynomial;  
}
```

The PhaseModel_t data structure will be defined as follows in the SIDS:

```
PhaseModel_t :=  
{  
List(char[33] Name1 ... NameNPZ); (r)  
List(float TemperatureLimitLower1 ... TemperatureLimitLowerNPZ); (r)  
List(float TemperatureLimitUpper1 ... TemperatureLimitUpperNPZ); (r)  
List(int NumberRanges1 ... NumberRangesNPZ); (r);  
List(RangeModel_t Range1 ... RangeNPZ); (r);  
}
```

The SpeciesModel_t data structure will be defined as follows in the SIDS:

```
SpeciesModel_t :=  
{  
int NumberSpecies; (r)  
List(float MolecularWeight1 ... MolecularWeightNS); (o)  
List(char[33] Name1 ... NameNS); (r)  
List(ElementalComposition_t StoichCoeff1 ... StoichCoeffNS); (r)  
List(int NumberPhases1 ... NumberPhasesNS); (r)  
List(PhaseModel_t PhaseData1 ... PhaseDataNS); (r);  
}
```

This construction allows the general storage of thermodynamic data used in most reacting flow models (CHEMKIN compatible). It is generalized to hold multiple phases for solid/liquids. For gaseous species there is a single instance of the phase. The number of ranges has been generalized to allow an arbitrary number of ranges (CEA compatible). The elemental composition is related through stoichiometric coefficients to the proposed ElementalModel_t data.