MODELING HYDRATES AND THE GAS HYDRATE MARKUP LANGUAGE

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ABSTRACT

Natural gas hydrates, as an important potential fuels, flow assurance hazards, and possible factors initiating the submarine geo-hazard and global climate change, have attracted the interest of scientists all over the world. After two centuries of hydrate research, a great amount of scientific data on gas hydrates has been accumulated. Therefore the means to manage, share, and exchange these data have become an urgent task. At present, metadata (Markup Language) is recognized as one of the most efficient ways to facilitate data management, storage, integration, exchange, discovery and retrieval. Therefore the CODATA Gas Hydrate Data Task Group proposed and specified Gas Hydrate Markup Language (GHML) as an extensible conceptual metadata model to characterize the features of data on gas hydrate. This article introduces the details of modeling portion of GHML.

Keywords: GHML, Model, Gas hydrate, Metadata

1   INTRODUCTION

The "Modeling" portion of GHML has assimilated information about gas hydrate modeling, consisting of such elements as name, purpose, main theories, and input/output parameters that are generally used in hydrate behavior modeling. The generation of this part of the GHML was essentially based on modeling software named "TOUGH-Fx/Hydrate," which is widely used for modeling gas hydrate resources. "TOUGH-Fx/Hydrate" is a good representative of the state-of-the-art model in this research field. Therefore, although the GHML used a single software program as a reference, elements abstracted from it are likely to be suitable for most applications.

During the development of this part, we consulted many other international metadata standards (Markup Languages) that provided good references to structure design, naming conventions, annotation format, etc. Consistency with these existing international standards ensures good communication and transferability between GHML and other international standard markup languages.

2   SCOPE

This standard specifies a conceptual data schema that defines the structure of a metadata/data instance for gas hydrate modeling. This conceptual data schema does not specify distribution, encoding, or means for use of this

standard that can be determined from other endorsed standards. In this standard, these characteristics of gas hydrate modeling may be divided into metadata category and data category. The standard can be used for gas hydrate data description, integration, management, and exchange not only by metadata producers but also by data managers.

3   STIPULATION

3.1   Base schema defines the data elements

Name - The name by which the data element is referenced.

Definition - The definition of the data element.

Datatype - Indicates the value's type (string, decimal, id, etc.) of an element.

MaxOccurs - The maximum permitted occurrence times of an element.

MinOccurs - The minimum permitted occurrence times of an element.

3.2   Naming convention

The naming convention in this standard is as follows:

(1) Element

The first letter of each concatenated word is capitalized, e.g.: InputParameter.

(2) Complex Type

Each complex type ends with "Type," and the first letter of each concatenated word is capitalized, e.g.: InputType.

(3) Simple Type and Attribute

The first letter is lowercase, and the first letter of each subsequent concatenated word is capitalized, e.g.: valueList.

3.3   XML schema and namespace

This standard uses XML Schema to define the GHML. XML Schema is a recommended metalanguage by W3C that can define data element, data type, value space, and element relations conveniently and clearly.

"Namespaces in XML" lets browsers interpret more than one XML-based language in a single document without confusing different elements with the same tag names. This standard defines the following namespaces:

targetNamespace = http://www.codata.org/ghml/

xmlns:ghml=http://www.codata.org/ghml

4   DETAILS OF MODELING ML SCHEMA

The basic structure of this portion of GHML is shown in Figure 1.
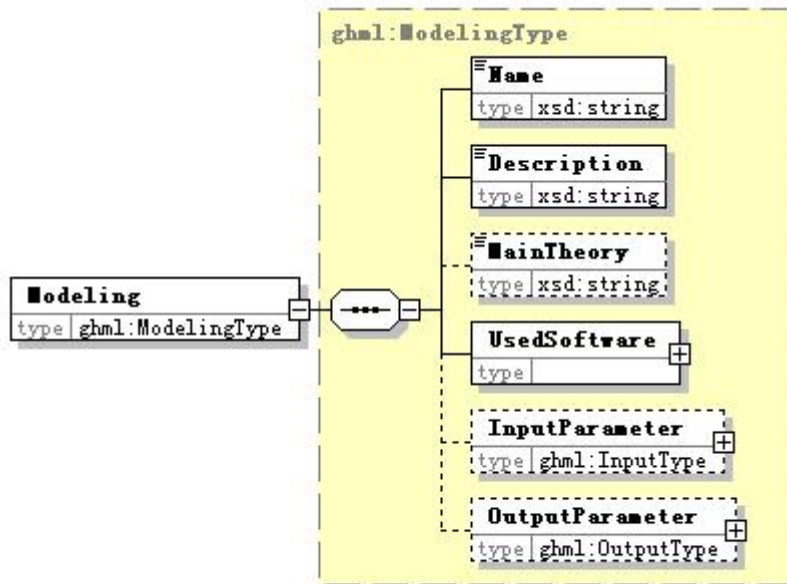
Figure 1. Basic Structure of Modeling Markup Language

This part of GHML consists of descriptive elements and data elements:

Descriptive elements:

- **Name[string]** - Name of this model.
- **Description[string]** - Some descriptive information (e.g. equation of state –EOS) and if an inhibitor is included, it should be mentioned by this element.
- **MainTheory[string]** - The main theory used in the model.
- **UsedSoftWare** - Includes two sub-elements: Name [string] -The name of the software with which the model was built. Version [string] -Version information of this software.

Data elements:

- **Input Parameter[ghml:InputType]:** This is one of the most important elements in this portion, which includes five complex elements, each of which answers one important modeling question (as shown as Figure 2).
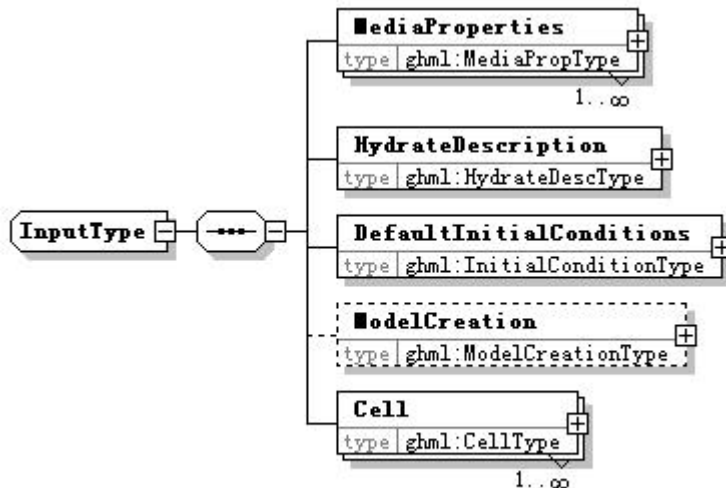
Figure 2. InputType

- ▪ **MediaProperties[MeidaPropType]** - A data block that lists all the parameters that describe the hydraulic, thermal and wettability properties of the geologic medium (Figure 3).
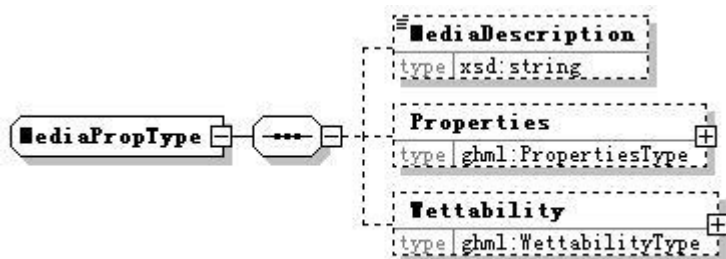

Figure 3. MediaPropType

- • **MediaDescription [string]** - Descriptive information about the media.
- • **Properties [ghml:PropertiesType]** - Physical and chemical properties of the media. This block includes such media properties as: **Density[double], Porosity[double], Permeability[double], WetHeatConductivity[double], SpecificHeat[double], and ThermalExpensivity[double].**
- • **Wettability [ghml:WettabilityType]** – Description of the porous media response as it is being wetted by fluids (Figure 4).
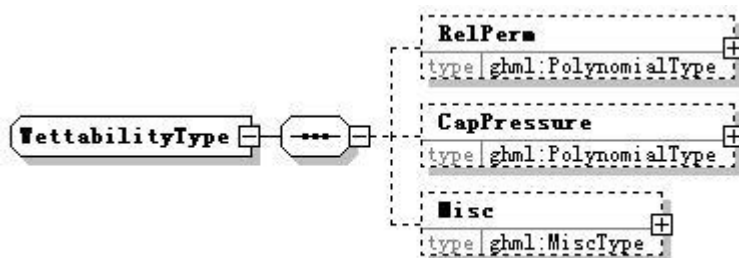

Figure 4. WettabilityType

- **RelPerm [ghml:PolynomialType]** - 3-phase relative permeability as a function of saturation. This element includes three sub-elements that describe the characteristics of the polymonial: **Polynomial [string]** , **CoefficientNumber[integer] -** The number of coefficients needed by the polynomial, and **Coefficient[double] -** Coefficient value.

- **CapPressure [ghml:PolynomialType] -** Capillary pressure. This element uses the same data type as **RelPerm** described above.

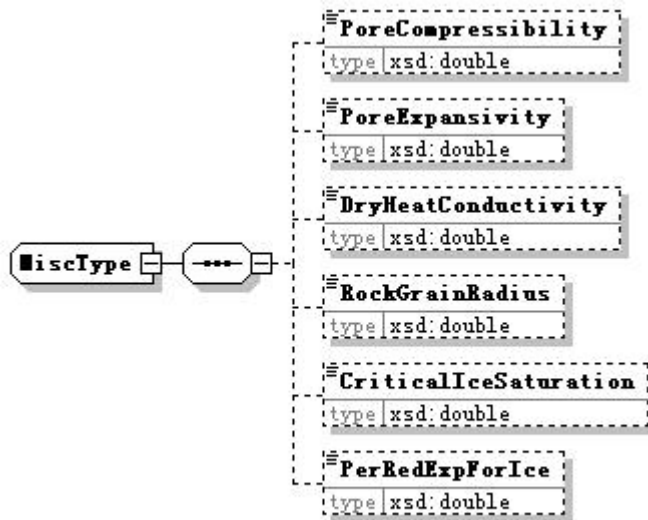- **Misc[ghml:MiscType]** – Miscellaneous material data (Figure 5).

Figure 5. MiscType

This element consists of:

- **PoreCompressibility[double]** - Defines how the pore volume changes as a function of pressure.
- **PoreExpansivity[double]** - How the pore volume changes with temperature.
  DryHeatConductivity[double] - Used with the wet heat conductivity to change the thermal conductivity of the rock.
- **RockGrainRadius[double]** - The radius of the rock grain.
- **CriticalIceSaturation[double]**
- **PerRedExpForIce[double]** - Permeability reduction exponent for ice.

- **HydrateDescription [HydrateDescType]** – Hydrate properties and behavior (Figure 6).
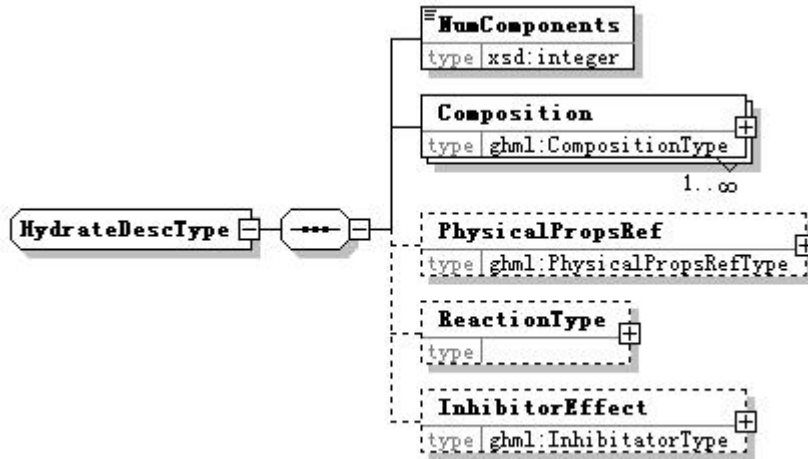
Figure 6. HydrateDescType

This element includes the following sub-elements:

- **NumComponents[xsd:integer]** - The number of components in a complex hydrate.
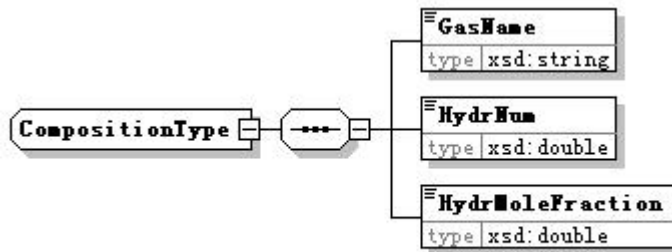- **Composition [ghml:CompositionType]** - Composition of the complex hydrate (Figure 7).

Figure 7. CompositionType

- **GasName[String]** - the name of the hydrate-forming gas.
- **HydrNum[double]** - the corresponding hydration number.
- **HydrMoleFraction[double]** - Hydrate mole fraction in the complex hydrate.
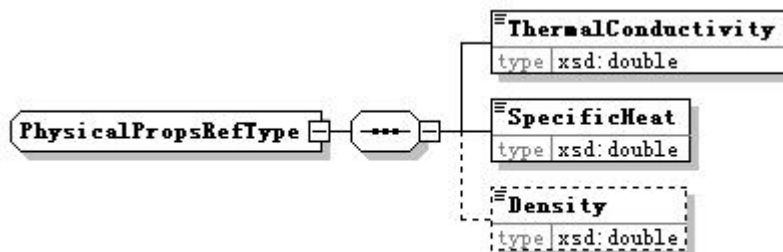- **PhysicalPropsRef[ghml:PysicalPropsRefType]** (Figure 8)

Figure 8. PhydicalPropsRefType

This block consists of three properties of hydrate**: ThermalConductivity [double], SpecificHeat[double],** and **Density[double].**

- **ReactionType** - Describes the type of hydrate reaction and may take one of two values. For simulations under equilibrium conditions, ReactionType is 'Equilibrium'. Kinetic hydrate reactions are considered when reaction type is Kinetic and tree parameters are needed at this circumstance: **ActivationEnergy[double]** - The activation energy for the hydrate dissociation [J/ mol]; **IntrinsicRate[double]** - Intrinsic hydration reaction constant K0 [kg/ (m^2. Pa.s)]; and **AreaFctor[double]-** Area adjustment factor [dimensionless].

- **InhibitorEffect[ghml:InhibitorType]** - Inhibitor-related data, which includes **TMaxOff [double]** - The inhibitor-induced reference temperature depression; **CMaxOff[double] -** Reference inhibitor mole fraction in the aqueous phase; **MWInhib[double]** - Molecular weight of the inhibitor [g/ mol]; **DInhib[double]** - Inhibitor density [kg/ m^3]; **HInhib[double] -** Specific enthalpy of inhibitor dissolution [kg/ m^3]; and **DifcoInhib[double]** - Diffusion coefficient of inhibitor in water [m^2/ s]

- **DefaultInitialCondition[DefaultInitialConditions]** - Default global initial conditions. Initial conditions are used to define the initial state of each cell. A hierarchy is used to determine the cell state. If defined at the cell, those values are used. If defined at the region, those are used. Finally, the default model initial conditions will be used. Default initial conditions are always defined for the model. This complex element consists of **PhaseType [string]** - Phase state of the modeling; **P [double]** – Pressure; **T [double]** – Temperature; **SH [double]** - Hydrate saturation; **SG [double]** - Gaseous phase saturations; **SA [double]** - Fluid phase saturations; **SI [double]** - Ice phase saturation; **Xinhibitor [double]** - Mole fraction of the inhibitor; and **XGasInWater [double]** - Mole fraction of gas in water.

- **ModelCreation[ModelCreationType]** - How the model was created (Figure 9).
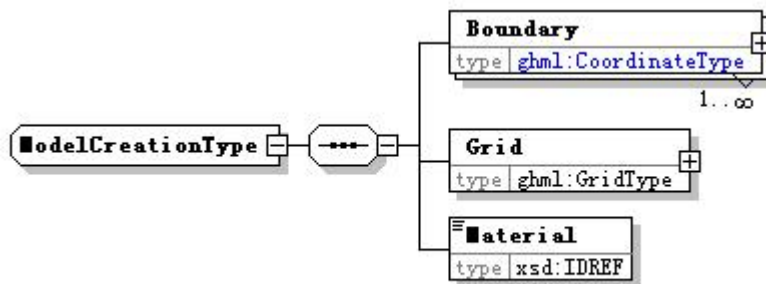

Figure 9. ModelCreationType

- **Boundary[CoordinateType] -** The first step in creating a model is to define the boundary. In this standard, we defined a common data type - **CoordinateType** to describe all coordinates elements that appear in this standard. CoordinateType consists of five elements: **X[double]; Y[double]; Z[double]; StrikeAzinuth[double]** -The degrees from North (the positive Y axis) in a clockwise direction; and **DipAngle [double]** - Degrees from horizontal of the plane.

- **Grid [GridType]** - Describes how the region is subdivided into sub-regions/cells by indicating the cell number in each direction of increasing coordinate. **XNumber [integer]** - cell number in X axis; **YNumber [integer]** - cell number in Y axis; and **ZNumber [integer]** - cell number in Z axis.
- **Material [IDREF]** - Indicates the material that adopted in the model.

▪ **Cell [CellType]** - Properties of a cell. Cells can be divided into two types: boundary cells and normal cells (Figure 10).
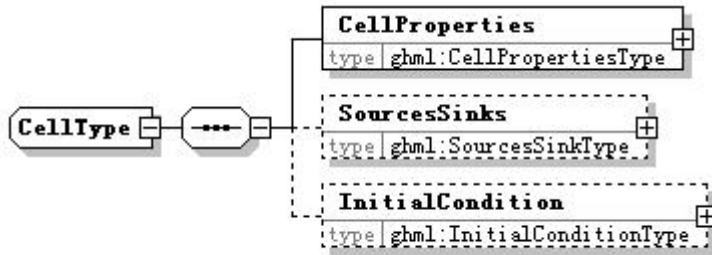

Figure 10. CellType

- **CellProperties[CellPropertiesType]** - Geometer properties of the cell (Figure 11).
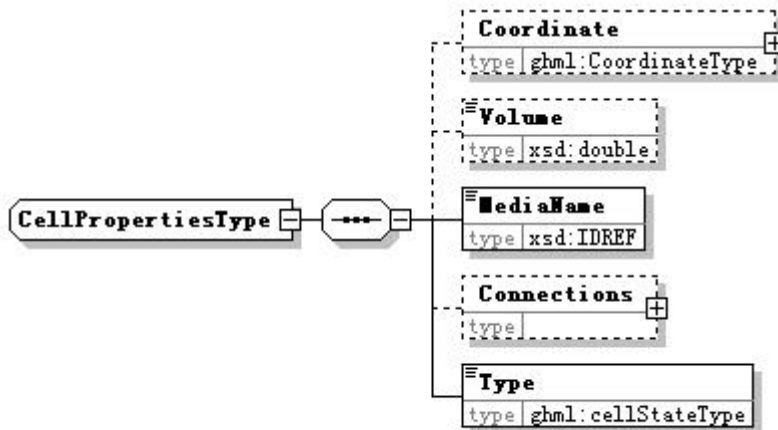

Figure 11. CellPropertiesType

▪ **Coordinate [ghml:CoordinateType]** – Described above.
▪ **Volume[double]** - Volume of the cell.
▪ **MediaName[IDREF]** - The media used in this cell.
▪ **Connections** - Common connection area over which the elements communicate/interact. This elements has three sub-elements: **Area [double]** - Interface area [m^2]; **D1[double]** and **D2[double]** - D1 and D2 refer to distance [m] from first and second element, respectively, to their common interface.
▪ **Type [ghml:cellStateType]** - Enumeration(Enabled, Disabled and Fixed State).

- **SourcesSinks[SourcesSinkType]** - Defines production from or injection into a cell (Figure 12).
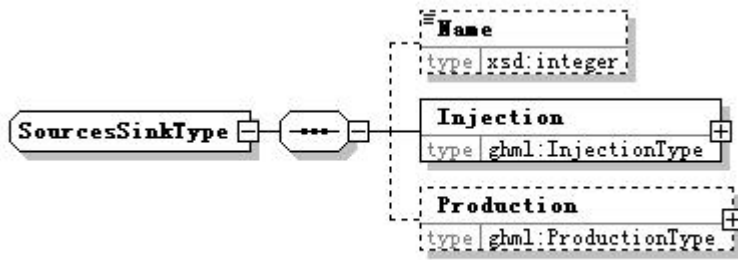

Figure 12. SourcesSinkType

- **Name[string]** - Name for the well.
- **Injection [ghml:InjectionType]** - Defines production injection into a cell. Injection parameters will vary depending on the EOS being used (Figure 13). In general, the user will specify a rate and an enthalpy for each component to be injected. The rates can be defined as constant (**Rate [double]** and **Enthalpy [double])** or using a table to give time/rate pairs.
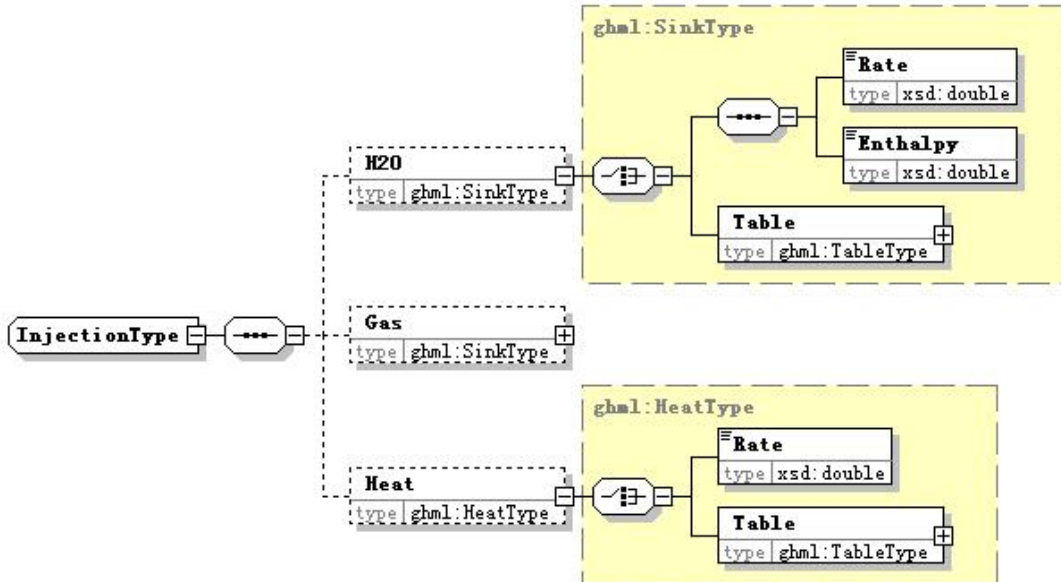

Figure 13. InjectionType

- **Production[ghml:ProductionType]** - Defines production from a cell.
- **Mass[ghml:HeatType]** - Defines the mass produced from the cell.

- **WellOnDeliv,** which includes two sub-elements: (**ProcuctivityIndex[integer]** and **Pressure[double])** - Define a boundary condition where the cell produces to a fixed pressure.
  - **InitialCondition[InitialConditionType]** - Defines the initial state of each cell, as described above.
- **OutputParameter[ghml:OutputType]** describes output parameters of the model (Figure 14). This element includes for complex sub-elements:
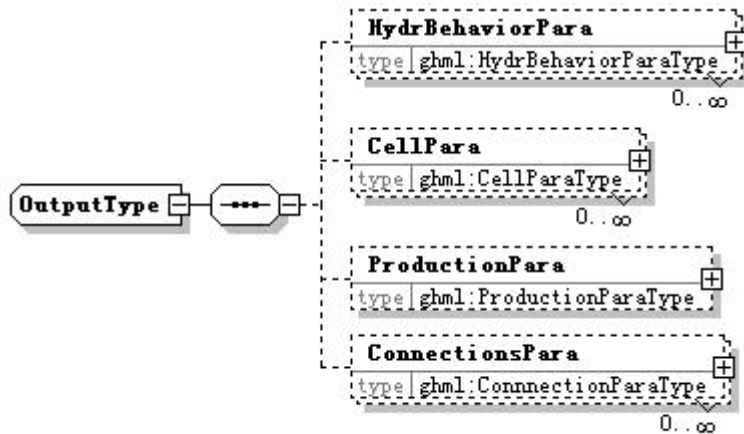

Figure 14. OutputType

- **HydrBehaviorPara[ghml: HydrBehaviorParaType] -** Output file that includes data describing the evolution of hydrate dissociation over time.
  - **Time[string]** - Simulation time.
  - **Cum_Release_MRate[double]** - Mass rate of CH_4 release from dissociation.
  - **Cum_ReleasTie_VRate[double]** - Volumetric rate of CH_4 release from dissociation.
  - **Cum_Rel_Mass[double]** - Cumulative mass of released gas from the entire domain from the beginning of the simulation.
  - **Cum_Rel_Volume[double]** - Cumulative volume of released gas from the entire domain from the beginning of the simulation.
  - **Free_Reservoir_Gas[double]** - Volume of free gas in the reservoir at the time of observation.
  - **Rem_Hydrate[double]** - Mass of hydrate remaining in the deposit at the time of observation.

- **ProductionPara[ghml:ProductionParaType]** - Data describing gas production (rates and production stream composition at wells)
  - **Time[string]** - Simulation time.
  - **Qm_CH4_prod[double]** Mass rate of CH_4 production.
  - **Qv_CH4 _prod[double]** -Volumetric rate of CH_4 production
  - **CumM_CH4_ prod[double]** - Cumulative mass of produced gas since the inception of the simulation.
  - **CumV_CH4_ prod[double]** - Cumulative volume of produced gas since the inception of the simulation.

- **Qm_H2O_prod[double]** - Mass rate of water production.
- **CumM_H2O_ prod[double]** - Cumulative mass of produced water since the inception of the simulation.

- **ConnectionsPara[ghml: ConnectionParaType]** - Output file that includes a list describing the evolution of connection-related parameters over time.
  - **Time [string]**
  - **HeatFlux[double]** - Heat flux .
  - **GasFlux[double]** - Gas flux.
  - **AquFlux[double]-**Liquid flux.
  - **Ch4inGas_flux[double]** - Flux of CH_4 in the gas phase.
  - **CH4inAqu_flux[double]** - Flux of CH_4 in the aqueous phase
  - **GasVeloc[double]** - Gas phase velocity.
  - **AquVeloc[double]** - Aqueous phase velocity.
  - **Gas_phi[double]** - Fugacity of the gas phase.
  - **Aqu_phi[double]** -Fugacity of the aqueous phase.

- **CellPara[ghml:CellParaType]** - Output file that includes a list describing the evolution of cell-related parameters over time.
  - **Time[string]**
  - **P[double]** – Pressure.
  - **T [double]** – Temperature.
  - **S_Hydrate[double]** - Hydrate saturation.
  - **S_gas[double]** - Gas saturation.
  - **S_aqu [double]** - Liquid saturation.
  - **S-Ice[double]** - Ice saturation.
  - **X_Inhibitor[double]** - Mass Fraction of inhibitor.
  - **P_CH4[double]** - Partial pressure of CH4.
  - **P_EqHydr[double]** - Equilibrium hydration pressure at temperature T.
  - **P_SatWar[double]** - Saturation pressure of water at temperature T.
  - **C_CH4inGas[double]** - Concentration of CH4 in the gas phase.
  - **C_CH4inAqu[double]** - Concentration of CH4 in the aqueous phase.
  - **Dens_Gas [double]** - Density of gas.
  - **Dens_Aqu [double]** - Liquid density.
  - **Dens_Hydr[double]** - Hydrate density.
  - **Visc_Gas [double]** - Gas viscosity.
  - **Visc_Aqu[double]** - liquid viscosity.
  - **Phi [double]** -Porosity.
  - **Pcap [double]** - Capillary pressures.
  - **Krel_Gas [double]** - Relative permeability of the gas phase.
  - **Krel_Aqu [double]** - Relative permeability of the aqueous phase.
  - **H_Gas [double]** - Enthalpy of the gas phase.
  - **H_Aqu [double]** - Enthalpy of the aqueous phase.
  - **H_Hydr [double]** - Enthalpy of the hydrate phase.

- **H_Ice [double]** - Enthalpy of the ice phase.
- **ReacTn_Rate[double]** - Rate of the hydration reaction.
- **Reactn_Heat[double]** - Heat of dissociation/formation.
- **T_shift** - Temperature shift in the hydration reaction caused by inhibitors.

5   REFERENCES

Dublin Core Metadata, Retrieved from the WWW, April 18, 2007: http://dublincore.org/.

Examples Using the PetraSim Pre- and Post-Processor for TOUGH-Fx/HYDRATE. Retrieved from the WWW, April 18, 2007: http://www.thunderheadeng.com/petrasim/manual_tetrad.pdf.

ISO 19115 Geographic information – Metadata. Retrieved from the WWW, April 18, 2007: http://www.iso.org/iso/en/CatalogueDetailPage.CatalogueDetail?CSNUMBER=26020&ICS1=35&ICS2=240&ICS3=70.

ThermoML – An XML-Based Approach for Storage and Exchange of Experimental and Critically Evaluated Thermophysical and Thermochemical Property Data. Retrieved from the WWW, April 18, 2007: http://trc.nist.gov/ThermoML.html.