Chemlogic:

A Logic Programming Computer Chemistry System

Second Edition

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* Abstract

Chemlogic is a logic program for computer chemistry that performs stoichiometric calculations, balances and completes equations, and converts between formulas and names. The program has applications in education, particularly as a study tool. Features are implemented using a chemical information database, linear equation solver, and grammatical rules. Guidance is provided for resolving errors in user input. Chemlogic is available on Android and the Web.

Background

In high school Chemistry, students learn to work with chemical compounds, equations and stoichiometric calculations. Algorithms were researched, adapted to chemistry problems and implemented in Prolog, to develop a program that could be used by both students and teachers.

Design and Implementation

User input is parsed into a form that can be easily manipulated and transformed. A parser recognizes a formal grammar describing valid user input. In Prolog, parsers are implemented using DCGs (Definite Clause Grammars), which provide a simplified syntax for creating logical clauses that process a grammar using difference lists, an efficient representation. [4]

Internal representations must be created for the parsed input. Chemlogic uses a pseudo-Abstract Syntax Tree to record the structure of an equation, as well as lists containing useful information (e.g. the elements contained in an equation).

The reaction type analysis module identifies common types of chemical reactions, predicts whether a reaction will take place, and completes chemical equations for common reactions, given the reactants. These features are implemented by matching the Abstract Syntax Tree generated by parsing an equation, against a pattern representing the structure of a certain chemical reaction type. In Prolog, this matching is performed by syntactic unification, which is the process of combining two structures by replacing variables with constant terms, so as to make the two structures equal.

Once the reaction type is determined, a prediction can be made as to whether the reaction will occur by comparing the relative positions in the reactivity series of the elements involved. The reaction type and the reaction prediction can then be displayed by the user interfaces, as additional information for the entered chemical equation.

To complete a chemical equation, the complete formulas of the product compounds must be calculated, given the arrangements of elements and ions determined by reaction pattern. This process is performed using rules specific to the type of compound being formed by the reaction. The complete formulas are then substituted into the equation structure, to produce a complete chemical equation. This structure can then be used as input by other modules, such as the chemical equation balancer.

Balancing of chemical equations is usually performed by inspection. [3] This process cannot easily be used in a program because it is unsystematic. Instead, Chemlogic uses an efficient algorithm, representing a chemical equation as a system of linear equations. One linear equation is created for every element in a chemical equation, with the number of occurrences of the element in each formula representing a coefficient, multiplied by an unknown

(the chemical equation coefficient). [5]

These systems are commonly solved by converting them to a matrix and applying Gaussian elimination. [2] In Chemlogic, a matrix is produced from structures created by the parser and lookup tables. The matrix is converted into a system of linear equations, which is then provided to the built-in CLP(q) facility, which can solve constraints over rational numbers. [1]

Stoichiometry is an important new feature of Chemlogic. The process of performing stoichiometric calculations begins by parsing a chemical equation that includes quantities for some compounds. Whenever a quantity is parsed, the number of significant figures in the value is determined and recorded in the quantity structure. A list of queries for quantities to be determined is also parsed.

The Abstract Syntax Tree for the given chemical equation is then traversed to determine the number of known quantities. If more than one quantity is known, the limiting reactant must be determined and used to calculate the results. This is performed by converting each known reactant quantity to moles (the standard unit for the amount of a chemical substance), then dividing by the corresponding coefficient of the reactant in the equation. The limiting reactant always has the lowest value for this ratio. If only one quantity is known, it must, logically, be used to perform all the calculations.

Once the correct quantity and compound to use as input for the calculation is determined, the list of queries is traversed, and the input quantity is converted to each requested output quantity. This calculation is performed according to the same method that is typically used when performing stoichiometric calculations manually. Unit conversions are performed by simple calculation rules, which take into account the maximum number of significant figures that can be yielded by the calculation.

Syntax errors cannot simply cause a program to fail — clear identification and explana-

tion of an error is necessary. When a predicate that must succeed for a given input to be valid fails, a syntax error exception is thrown, containing a code name for the error and the remaining unparsed input (within the tail). The exception handler attempts to localize the error by highlighting only the erroneous part of the tail, using rules specific to the type of the first character.

The Android App was developed to make Chemlogic more readily available as a study tool. The App consists of a user-interface, implemented in Java, using the Android APIs, and a package consisting of the cross-compiled code of Chemlogic and its dependencies. The user interface communicates with Chemlogic through a UNIX pipe. Upon receiving the solution from Chemlogic, the interface renders the formatting of the result and displays it.

The Chemlogic package contains a copy of the Chemlogic command-line interface, compiled as a stand-alone application with an embedded Prolog interpreter in its binary, some necessary Linux libraries and an initialization script. When loaded, the App executes the initialization script, which starts Chemlogic by running the dynamic linker to locate and link Chemlogic with the provided libraries.

Discussion

Prolog was chosen as the language for Chemlogic because its features make it well suited to writing programs of this type in a simple and efficient way. The built-in Definite Clause Grammars syntax allows a programmer to implement advanced parsers using a very simple syntax, and strong support for metaprogramming allows syntax and code to be simplified in powerful ways. Using a logic programming language, such as Prolog, enables the programmer to describe the results, instead of the process. [7]

Performance was analyzed in Chemlogic by counting inferences (provided by `time/1`) used by different algorithms for various problem sizes. Algorithms were compared on their

fixed inferences (intercept), inferences per item (slope) and to ensure that their complexities were not exponential.

Further research and development — The parsers currently implemented in Chemlogic process user input directly, as character lists, without a tokenization process. Using new features available in version 7 of SWI-Prolog, a simple and fast procedure could be implemented to separate user input into space-delimited parts, [8] significantly reducing the number of tests and operations required to perform parsing.

Developing a feature to automatically generate and mark random chemistry problems for student review and test creation would be an important extension to Chemlogic. With the addition of reaction type analysis, the preliminary development for this feature has been completed. The reaction type, equation, formula and name grammars in Chemlogic could be extended to produce random valid structures, in addition to simply recognizing and converting them.

Conclusions

Each module of Chemlogic is designed to transform the standardized Abstract Syntax Trees generated by the parsers, allowing for modules to be composed together, each adding a piece of functionality as structures are passed from predicate to predicate. In this way, existing modules can make use of new functionality, new features can be implemented based on existing calculations and structures, and modules can be connected to as part of integrated user interfaces.

Chemlogic was successfully extended to implement new features, based upon the existing modular structure, and can now perform stoichiometric calculations, convert chemical quantities between units, and complete chemical reactions. The balancing and formula to name conversion features were further developed and made available in a mobile application for Android.

Earlier Work

The original version of Chemlogic was an experimental program I developed in 2012, to simplify my Science homework.

Based on these experiments, the project was extended in 2013 and 2014. The program was rewritten in Prolog, new algorithms were studied and adapted and many new features were implemented. The current modular design and structure of Chemlogic was implemented in Version 1, which supported balancing chemical equations, converting chemical names to formulas, and vice-versa. This version was presented at the 2014 CWSF in Windsor, where it received a Bronze Excellence Award.

In 2014 and 2015, Chemlogic was further developed to significantly expand the project, by continuing to improve existing features, adding a new user interface and adding support for higher levels of high school Chemistry. Version 2 of Chemlogic introduced the Android user interface and support for stoichiometric calculations, chemical unit conversions and reaction type analysis.

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Obtaining Chemlogic / Contact

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Chemlogic is open-source software. A copy of the program and additional information is available at http://icebergsys.ca/chemlogic

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