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Thermosteam: BioSTEAM's Premier Thermodynamic Engine

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Summary

`Thermosteam` is a thermodynamic engine capable of solving mass and energy balances, estimating mixture properties, solving thermodynamic phase equilibria, and modeling stoichiometric reactions. All chemical data in `Thermosteam` is imported from the `chemicals` library (C. Bell & contributors, 2020), an open-source compilation of data and functions for the estimation of pure component chemical and mixture properties. `Thermosteam`'s fast and flexible platform has enabled the evaluation of conceptual and emerging biochemical production processes. The Biorefinery Simulation and Techno-Economic Analysis Modules (BioSTEAM) — capable of modeling reactors, distillation columns, heat exchangers, and other unit operations — has adopted `Thermosteam` as its premier thermodynamic engine (Cortés-Peña et al., 2020). Published biorefinery designs modeled in BioSTEAM implement thermodynamic property packages created with `Thermosteam` (BioSTEAM Development Group, 2020), including a cornstover biorefinery for the production of cellulosic ethanol, a lipid-cane biorefinery for the co-production of ethanol and biodiesel, and a wheatstraw biorefinery for the production of cellulosic ethanol (Cortés-Peña et al., 2020; Sanchis-Sebastiá et al., 2020).

Statement of Need

The overarching goal of `Thermosteam` is to aid the rigorous design and simulation of chemical production processes, whereby low value feedstocks are converted to high value products via chemical reactions and thermodynamic-driven separations. For example, modeling the separation of volatile chemicals from heavier ones in a distillation column (e.g., distilling ethanol from water), requires vapor-liquid phase equilibrium calculations to predict how well volatile chemicals selectively partition into the vapor phase. Additionally, fluid viscosities, densities, and surface tensions are required to appropriately design a distillation column that can achieve a specified recovery of chemicals (Green, 2018).

Several open-source libraries in Python have comparable capabilities to `Thermosteam` in the estimation of fluid properties and phase equilibria: most notably `Cantera` and `CoolProp`. `Cantera` is a collection of software tools capable of modeling kinetic reactions, thermodynamic equilibrium, and mixture properties (Goodwin et al., 2018). `Cantera`'s built-in chemicals are limited to 8, but new chemicals can be defined by users with flexibility on the amount of detail. `Thermosteam` has yet to implement any features on kinetic reaction networks, but exposes a larger set of roughly 20,000 built-in chemicals from the `chemicals` library. Users may also define new models and pseudo-chemicals that are compatible with all of `Thermosteam`'s features. `CoolProp` offers fast and accurate thermodynamic and transport properties for 122 chemical components, and can estimate phase equilibrium and mixture properties (I. H. Bell et al., 2014). `CoolProp` also offers an interface to the NIST REFPROP software, which is

considered the gold standard in thermophysical properties (Lemmon et al., 2018). It is within Thermosteam's roadmap to use CoolProp as part of its built-in models. While CoolProp focuses on thermophysical chemical properties, Thermosteam also includes mass and energy balances and stoichiometric reactions as one of its central features.

Roadmap

The main development items in Thermosteam's roadmap concerns the implementation of fast, robust, and accurate algorithms for estimating mixture properties and solving thermodynamic phase equilibria. Through Thermosteam, BioSTEAM is able to evaluate a range of biofuels and bioproducts, but further efforts on these development items would enable the evaluation of a broader portfolio of potential bioproducts.

In Thermosteam, Peng Robinson is the default equation of state for all pure components. However, the estimation of pure component chemical properties is not limited to solving the equation of state. Several models of thermodynamic properties (e.g., density, heat capacity, vapor pressure, heat of vaporization) are correlations that rely on fitted coefficients and key chemical properties (e.g., critical temperature and pressure). To facilitate the calculation of mixture properties, Thermosteam's mixing rule estimates mixture properties by assuming a molar weighted average of the pure chemical properties. However, Thermosteam aims to implement rigorous equation of state (EOS) mixing rules for the estimation of mixture properties.

Thermosteam allows for fast estimation of thermodynamic equilibrium within hundreds of microseconds through the smart use of cache and Numba just-in-time (JIT) compiled functions (Lam et al., 2015). The main vapor-liquid equilibrium (VLE) algorithm solves the modified Raoult's law equation with activity coefficients estimated through UNIQUAC Functional-group Activity Coefficients (UNIFAC) interaction parameters (Jürgen Gmehling et al., 2019). Modified Raoult's law is suitable to estimate VLE of nonideal mixtures under low to moderate pressures. At high to near-critical pressures, gaseous nonidealities become more significant. In a near future, Thermosteam may also implement the Predictive Soave–Redlich–Kwong (PSRK) functional group model for estimating phase equilibrium of critical mixtures.

All of Thermosteam's application program interface (API) is documented with examples. These examples also serve as preliminary tests that must pass before accepting any changes to the software via continuous integration on Github. Additionally, the online documentation includes a full tutorial that concludes with the creation of a property package. Thermosteam's powerful features and extensive documentation encourage users to become a part of its community-driven platform and help it become more industrially and academically relevant.

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References

Bell, C., & contributors. (2020). Chemicals: Chemical properties component of chemical engineering design library (ChEDL). In *GitHub repository*. GitHub. https://github.com/CalebBell/chemicals

Bell, I. H., Wronski, J., Quoilin, S., & Lemort, V. (2014). Pure and pseudo-pure fluid thermophysical property evaluation and the open-source thermophysical property library CoolProp. *Industrial & Engineering Chemistry Research*, *53*(6), 2498–2508. https://doi.org/10.1021/ie4033999

Cortés-Peña, Y., Kumar, D., Singh, V., & Guest, J. S. (2020). BioSTEAM: A fast and flexible platform for the design, simulation, and techno-economic analysis of biorefineries under uncertainty. *ACS Sustainable Chemistry & Engineering*, *8*(8), 3302–3310. https://doi.org/10.1021/acssuschemeng.9b07040

Goodwin, D. G., Speth, R. L., Moffat, H. K., & Weber, B. W. (2018). *Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes* (Version 2.4.0) [Computer software]. Zenodo. https://doi.org/10.5281/zenodo.1174508

Green, D. W. (2018). Distillation. In *Perry's chemical engineers' handbook 9th edition* (9th ed.). McGraw-Hill Education. ISBN: 978-0-07-183408-7 978-0-07-183409-4

Jürgen Gmehling, Michael Kleiber, Bärbel Kolbe, & Jürgen Rarey. (2019). *Chemical thermodynamics for process simulation* (pp. 173–321). Wiley. ISBN: 978-3-527-34325-6

Lam, S. K., Pitrou, A., & Seibert, S. (2015). Numba: A LLVM-Based Python JIT Compiler. *Proceedings of the Second Workshop on the LLVM Compiler Infrastructure in HPC*. https://doi.org/10.1145/2833157.2833162

Lemmon, E. W., Bell, I. H., Huber, M. L., & McLinden, M. O. (2018). *NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, Version 10.0, National Institute of Standards and Technology*. https://doi.org/10.18434/T4/1502528

Sanchis-Sebastiá, M., Gomis-Fons, J., Galbe, M., & Wallberg, O. (2020). Techno-Economic Evaluation of Biorefineries Based on Low-Value Feedstocks Using the BioSTEAM Software: A Case Study for Animal Bedding. *Processes*, *8*(8), 904. https://doi.org/10.3390/pr8080904

BioSTEAM Development Group. (2020). Bioindustrial-park: BioSTEAM's premier repository for biorefinery models and results. In *GitHub repository*. GitHub. https://github.com/BioSTEAMDevelopmentGroup/Bioindustrial-Park