BRC Science Highlight
December 2020

Thermosteam: BioSTEAM's Premier Thermodynamic Engine

Objective

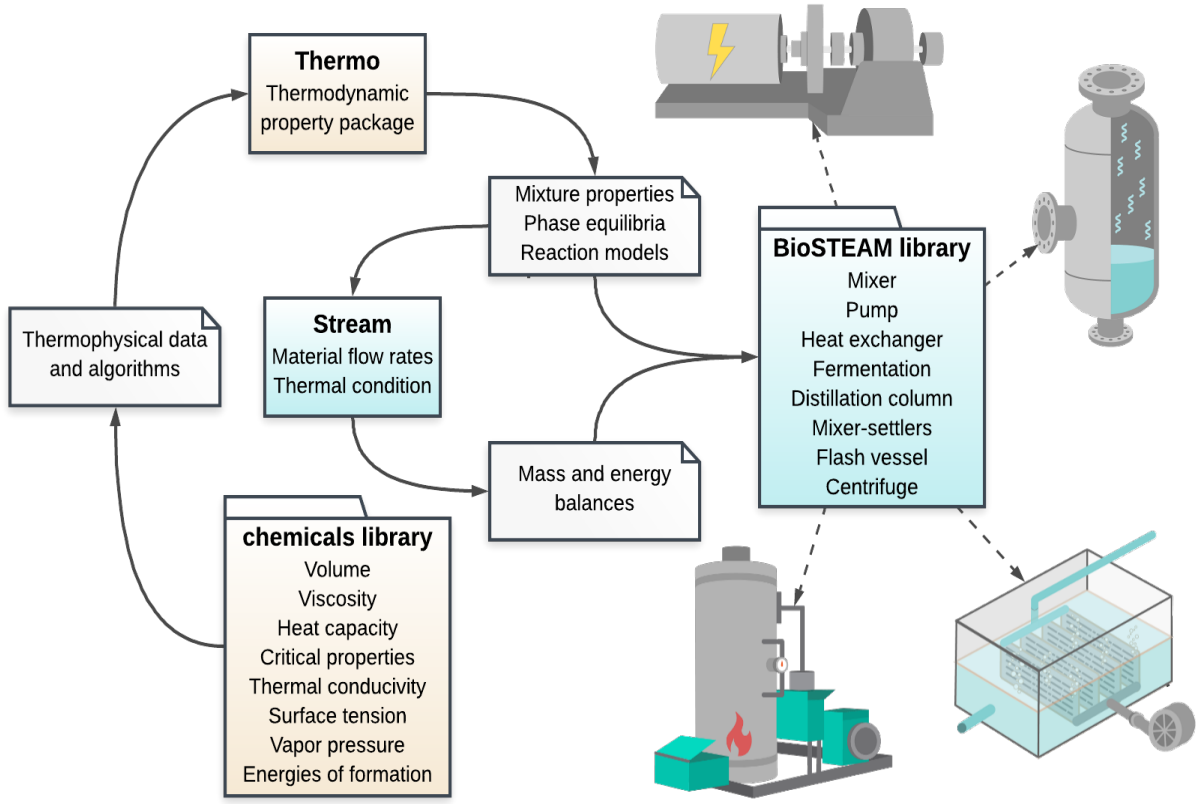
The capacity to conduct rigorous, robust techno-economic analysis (TEA) will be critical to strategically chart a course for the emerging bioeconomy. The recently published Biorefinery Simulation and Techno-Economic Analysis Modules (BioSTEAM)[1] is an open-source, steady-state process simulation library for biorefinery design, simulation, and TEA. Here, we introduce Thermosteam[2], the thermodynamic engine that enables rigorous design and simulation of unit operations in BioSTEAM.

Approach

- Integration with existing chemical library to incorporate 20,000 built-in chemicals, with the option to define pseudo-chemicals to meet user needs.
- Rapid and robust algorithms for estimating mixture properties and phase equilibria.
- Rapid estimation of thermodynamic equilibria within hundreds of microseconds using just-in-time compiled functions.

Results

Thermosteam can accurately solve mass and energy balances, estimate mixture properties, solve thermodynamic phase equilibria, and model stoichiometric reactions.



Thermosteam creates thermodynamic property packages that directly feed into BioSTEAM for the rigorous design and simulation of unit operations.

Significance

Through Thermosteam, BioSTEAM can be used to evaluate a range of biofuels and bioproducts. Further development of Thermosteam would enable the evaluation of a broader portfolio of potential bioproducts.

[1]*Cortes-Peña et al. 2020. "BioSTEAM: A Fast and Flexible Platform for the Design, Simulation, and Techno-Economic Analysis of Biorefineries Under Uncertainty."* ***ACS Sustainable Chemistry and Engineering****. DOI:10.1021/acssuschemeng.9b07040*

[2]*Cortés-Peña, 2020. "Thermosteam: BioSTEAM's Premier Thermodynamic Engine."* ***The Journal of Open Source Software****.* DOI:10.21105/joss.02814

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CENTER FOR ADVANCED BIOENERGY AND BIOPRODUCTS INNOVATION
U.S. DEPARTMENT OF ENERGY