A MILP Mathematical Formulation to Apply Total Site Analysis for the Synthesis of Biorefineries

Konstantinos A. Pyrgakis, Antonis C. Kokossis
National Technical University of Athens, School of Chemical Engineering,
Zografou Campus 15780, Greece

Biorefineries constitute the most promising routes for the establishment of a viable biobased economy that focuses on the replacement of fossil-oil with biorenewable sources in any application of materials and energy production. Whereas 1st generation biofuels quickly abate, 2nd generation production is taking off in Europe, US, China and South America focusing on the replacement of fossil transportation fuels. Demos, pilot plants and lighthouse projects further focus on bio-processing techniques to incorporate biomass based value-added chemicals in existing or future industry. Biorefining of biomass, through both thermochemical and biochemical paths, generates a wide range of chemicals (fibre materials, plastics, polymers, surfactants, solvents, lubricants, bulk chemicals and chemical specialties, pharmaceuticals and cosmetics) through large and complex value chain paths. The multiplicity of biomass supplies and chemicals provide strong incentives for the development of multi-product biorefineries. Under these conditions, multiple biorefining infrastructures emerge through value chains that need to be evaluated and optimized. The crucial challenge concerning the development of future biorefineries is the selection and integration of the appropriate biomass conversion processes that secure optimal efficiencies in the use of materials and energy composing sustainable bio-product portfolios.

Energy consumption, with a great impact on economical viability of biorefinery plants, should be targeted in the core of the synthesis problem. Energy integration constitutes a powerful tool that detects the maximum feasible and sustainable margins of energy efficiency. The need to energy integrate multi-product plants naturally relates to Total Site Analysis (TSA); a Pinch Analysis tool successfully applied in Oil & Gas industry. Nevertheless, TSA has been exclusively applied in plants with fixed processes. To the contrary, biorefineries hold the processes as degrees of freedom, since they involve processes that are possible to enter the final plant, and the analysis is then called to tackle a combinatorial problem.

In these cases, the conventional thermodynamic approach would require the repeating application of graphical tools to integrate involved processes for each possible plant and ranking of multiple combinations to detect the best one. Moreover, the potential combinations even explode as the number of chemicals increase, consequently making the exhaustive application of thermodynamics counter effective. Instead, the proposed approach combines thermodynamics with mathematical programming to screen and integrate the candidate processes using a heat cascade representation that is formulated as a discrete-continuous optimization problem. As a result, Total Site Analysis has been upgraded into a process synthesis tool capable to evaluate and valorize integration potential among candidates and detect product portfolios that benefit the utmost from their collocation highlighting promising energy synergies. An extended MILP transshipment model is proposed to apply TSA with the capacity to address the additional degrees of freedom (chemical paths) aiming to synthesize the biorefinery plant that subjects to minimum energy consumption.

The proposed mathematical model has been applied in the courses of a real life biorefinery case to assess a set of 7 competitive processes that are possible to get integrated together with a core process that fractionates lignocellulosic biomass into three intermediate chemicals: C5 Sugars, C6 Sugars and Lignin. The 7 competitors are possible to valorize the three intermediates generating up to 41 different plants. The optimization approach is required to screen the multiple combinations and select the best product portfolio. The energy savings associated with the selected portfolio range to 138 MW of hot utilities (steam) and 138 MW of cold utilities (cold water and refrigeration). The utility savings reached

78% (hot) and 87% (cold), while improvements over the stand-alone integration ranged up to 14%. The optimization approach has been also applied to find alternative promising portfolios with savings ranging from 78% to 88%.