RESUMEN

La producción sustentable de energía constituye uno de los desafíos más importantes del presente siglo. En particular, la producción de biocombustibles, basados en materias primas renovables, requiere aún de esfuerzos de investigación a nivel celular, de procesos y de plantas completas, para lograr competitividad económica frente a los combustibles fósiles.

En la presente tesis, se proponen modelos matemáticos de creciente complejidad y se aplican metodologías de programación matemática avanzada para la resolución de problemas de diseño y optimización de procesos de producción de biocombustibles. Se formulan modelos matemáticos que describen desde la red metabólica de una cianobacteria hasta una planta completa de producción de bioetanol, considerando también procesos de extracción y deshidratación de etanol con fluidos supercríticos y procesos de fermentación discontinuos para la producción de hidrógeno. En este sentido, este trabajo analiza, en primer lugar, una planta de producción de etanol a partir de granos, en particular, sorgo granífero, una materia prima disponible en la región sudoeste de la provincia de Buenos Aires y La Pampa. Se trata de una tecnología madura, que resulta de interés a nivel regional y nacional. Se formulan balances de masa y energía para el proceso y se realiza una evaluación económica de una planta basada en la tecnología de molienda seca. A continuación, y con el objetivo de realizar aportes en el diseño de redes metabólicas para la producción sustentable de etanol, se propone un modelo matemático para una cianobacteria modificada genéticamente para producir etanol. Un punto importante es que en este caso la fuente de carbono no es glucosa, sino dióxido de carbono que se puede obtener de una corriente residual. Se formulan problemas de programación lineal mixto entera (MILP) en dos niveles y se propone una reformulación para la maximización simultánea del crecimiento celular y la producción de etanol, con resultados comparables a los reportados por una empresa

que aplica esa tecnología. Asimismo, se presentan modelos rigurosos para la etapa final del proceso de producción de etanol: la deshidratación mediante un proceso de extracción con fluidos supercríticos, considerando diversas alternativas de integración energética, en un marco de optimización económica. Esta tecnología resulta altamente competitiva con las actuales tecnologías comerciales.

Finalmente, se proponen modelos dinámicos de procesos de producción de biohidrógeno mediante consorcio de bacterias, en un bio-reactor discontinuo, y se estiman los principales parámetros cinéticos, basados en datos experimentales obtenidos para tal fin.

ABSTRACT

Sustainable energy production constitutes a main challenge within this century. In particular, biofuel production, which is based on renewable raw materials, still requires increased research efforts at cellular, process and plant levels to be economically competitive with fossil fuel production.

In this work, mathematical models of increasing complexity are proposed for the design and optimization of biofuel production processes. Advanced mathematical programming techniques are applied for describing processes going from the metabolic network of a cyanobacterium to an entire ethanol plant, including extraction processes with supercritical fluids for ethanol dehydration and discontinuous fermentation processes for hydrogen production.

As a first step, an ethanol plant based on grain sorghum is analyzed. This cereal is widely available in Buenos Aires and La Pampa provinces. Even though it is a mature technology, it is of regional and national interest. Mass and energy balances are formulated and an economic evaluation is carried out for a dry mill technology.

To analyze a more sustainable alternative, a mathematical model is proposed for a genetically modified cyanobaterium producing ethanol. The important issue in this case is that the carbon source is no longer glucose but carbon dioxide that can be obtained from a residual stream. Mixed integer linear programming problems are formulated for the simultaneous maximization of cellular growth and ethanol production. The bilevel optimization problem is reformulated to a single level one, using duality theory concepts. Ethanol yields are comparable to experimental values reported by a commercial plant based on this technology.

In the following step, rigorous models are proposed for energy integration and economic optimization of the ethanol dehydration step, through extraction with supercritical fluids. This technology turns out to be competitive with current commercial ones.

Finally, dynamic kinetic models are proposed for hydrogen production through bacteria consortium in a batch fermentor, based on residual streams. Main kinetic parameters are determined by solving a dynamic parameter estimation problem based on experimental data for this process.

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