Infinite DimEnsionAl State-space
as a Systematic Process Intensification Tool:
Energetic Intensification of Hydrogen Production

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ABSTRACT:

In this work, process intensification is identified as a process synthesis activity seeking significant improvements over traditional designs. The Infinite-DimEnsionAl State-space (IDEAS) conceptual framework is proposed as a systematic process intensification tool, which can identify intensified process designs, and assess fundamental performance limitations of networks of technologies under consideration. The synthesis of intensified flowsheets, in an energy efficiency sense, is pursued through the simultaneous synthesis of the flowsheet and its heat exchange network. The use, for the first time in process synthesis, of atomic balance, and Gibbs free energy minimization based equilibrium reactor models, enables a broad state-space search for process intensification opportunities, even by low dimensional, feasible, linear programming, IDEAS approximations. Application of the proposed method to natural gas reforming based hydrogen production, identifies intensified process designs featuring hot utility costs that can be lower by over an order of magnitude to those of traditional designs.

INTRODUCTION:

The academic development of the Chemical Engineering profession was first focused on Process Analysis. For decades, researchers developed first principle based models aiming to capture the behavior of chemical processes¹⁻². The continuous improvement of computer technology, combined with advances in model simulation methods, has enabled the repeated ad-hoc use of these process analysis methods in chemical process design. Process Synthesis methods have also begun to appear (including an early book on the subject³), on a variety of synthesis problems: Solvay cluster synthesis⁴⁻⁵, heat integration⁶⁻¹², mass integration¹³, distillation network synthesis¹⁴⁻¹⁶ and reaction attainable region based synthesis¹⁷⁻²³. Roger Sargent pioneered the development of several process synthesis methods. As an example, his work with Westerberg on SPEED-UP²⁴, Gaminibandara on distillation¹⁴, and Grossmann on heat exchange network synthesis²⁵, established algorithmic and optimization based approaches to process synthesis as a major direction in the field. In his prophetic paper²⁶, Sargent highlights important directions in unconstrained optimization (e.g. Davidon-Fletcher-Powell, rank-one for robust convergence, conjugate gradient Fletcher-Reeves for reduced data storage), constrained optimization with nonlinear equality or inequality constraints (generalized-reduced-gradient, variable metric projection), and problems involving discrete variables (integer programming) where he identifies branch and bound as the only practical method (at the time), albeit providing caution that “the computation and storage problems rapidly get out of hand for all but the smallest problems.” Mixed integer nonlinear programs (MINLP’s), and non-smooth optimization formulations, have indeed been used more recently for the synthesis of heat-integrated flowsheets (using pinch analysis)^{15,27-28} and the simultaneous synthesis of flowsheets and their associated heat exchange networks²⁹, although Sargent’s prediction prophetically

remains valid. Infinite dimensional linear programming formulations to the synthesis of heat-integrated flowsheets (using pinch analysis)³⁰, and the simultaneous synthesis of flowsheets and their associated heat exchange networks³¹, have been presented, and constitute the conceptual foundation of this work.

Process intensification is a strategy for making dramatic reductions (order 100 or more) in the size of a chemical plant that attains given production objectives³². These reductions can come from reducing the number of units employed in the chemical plant as well as decreasing the size of individual units. Expanding the scope of process intensification beyond size has led to its characterization as “any chemical engineering development that leads to substantially smaller, cleaner, and more energy efficient technology”³³. Focusing on chemical engineering developments related to process synthesis, Stankiewicz³⁴ refers to the methyl acetate process by Eastman Chemical³⁵ as “widely regarded as a textbook example of process intensification”, wherein “task analysis-based process synthesis resulted in the replacement of traditional reactors and separation units by a highly integrated reactive distillation column”. Indeed, this patented process³⁶ employs only three major pieces of equipment, as opposed to the traditional manufacturing process, which employs twenty-eight major pieces of equipment. This kind of reactor and separation unit replacement by highly integrated reactive distillation column equipment³³ has been pursued using such process synthesis tools as residue curve maps^{37,38}.

In Moulijn’s and Stankiewicz’s book on process intensification³⁹ process synthesis is considered to be a process intensification method worthy of a chapter (11), which “focuses on the application of *process synthesis* principles to the optimal design of integrated chemical processing plants”. In the first chapter of that same book, Stankiewicz and Drinkenburg⁴⁰ identify process synthesis as a software method that is a part of the process intensification

toolbox, and state that “Process synthesis is in some sense a sister discipline of process intensification”. More recently, Moulijn et al⁴⁰ identify process systems engineering as a “chemical engineering skill” that supports process intensification, when process intensification is “considered as the technical objective.” They also state “This paper aims to ... explore and activate the interface between process systems engineering (PSE) and PI.” The above combined with the statements of Stankiewicz³⁴ on the methyl acetate process, and Siirola³⁵ “process synthesis is the invention of flowsheet alternatives at conceptual design stage of the innovation process”, lead us to conclude that any process synthesis activity that attains *significant* improvements over existing process designs can be classified as process intensification. This realization, reinforced by the suggestion of Moulijn et al⁴¹, that “a distinction needs to be made between PI as an *objective* for process development and design and PI as a scientific *skill* area”, leads us to pursue the development of systematic process intensification tools within the process synthesis toolbox through the intensification of process networks rather than just process equipment.

The Infinite Dimensional State-space (IDEAS) framework is a process synthesis methodology that can serve as a systematic process intensification tool. When process synthesis is carried out, it is not known a-priori whether significant improvements can be attained over a baseline design, that would subsequently justify the characterization of the synthesized process as an intensified process over its baseline counterpart. IDEAS can serve as a process intensification tool since, unlike other synthesis methods, it does not require an a priori pre-determined network structure as a starting point for its implementation. As a result, IDEAS can arrive at truly innovative designs, since it does not encompass designer preconceptions into its methodology. IDEAS can also identify fundamental limitations to the level of performance

attainable by any particular technology or combination of technologies, without any a priori commitment to any particular design. If these performance limits are close to the performance of existing known designs, then process intensification is not feasible based on the technology (technologies) under consideration, and additional/alternative technologies must be considered. If, on the other hand, IDEAS (or even low dimensional IDEAS approximations) can identify designs whose performance represents a significant improvement over the performance of known designs, then IDEAS is validated as a systematic process network intensification tool.

The remaining article is structured as follows: The IDEAS formulation to process flowsheeting is presented, including a property that enables the applicability of IDEAS to the employed reactor models. Next, an illustrative case study is presented, in which the IDEAS conceptual framework is employed as a tool in identifying intensified process flowsheets for natural gas reforming based hydrogen production. Finally, the obtained results are discussed, and conclusions are drawn.

IDEAS MATHEMATICAL FORMULATION OF PROCESS FLOWSHEETING:

The IDEAS framework decomposes a process network into an operator network (OP), where the unit operations (reactors, separators, heat exchangers, etc.) occur, and a distribution network (DN), where the flow operations (mixing, splitting, recycling, and bypass) occur. IDEAS represents a paradigm shift which establishes that chemical process nonlinearities need not be manifested during flowsheet optimization, but rather can be fully accounted for prior to optimization. Within the IDEAS framework, the optimal process network synthesis problem is formulated as an infinite linear program (ILP), whose solution is approximated by finite-dimensional linear programs of ever-increasing size. It should be noted that the IDEAS infinite dimensional linear programming (ILP) formulation identifies the synthesis problem's global

optimum, while the IDEAS finite dimensional linear programs represent approximations of the global optimum that can identify intensified process designs.

IDEAS has been successfully applied to numerous globally optimal process network synthesis problems, such as mass-exchange network synthesis,⁴² complex distillation network synthesis,^{30,43} power cycle synthesis,³¹ reactor network synthesis,^{44,45} reactive distillation network synthesis,⁴⁶ separation network synthesis,⁴⁷ attainable region construction,^{48–51} and batch attainable region construction⁵². More recently, the IDEAS framework has been used to incorporate efficiency considerations, which constitute one of the criteria employed in the expanded definition of process intensification⁵³, in reactor network synthesis, by minimizing the network's entropy generation. In particular, it has been shown that the entropy generation and energy consumption of isothermal, isobaric reactor networks only depend on the network's inlet and outlet stream compositions and flow rates, and are independent of the network structure, as long as the universe of realizable reactor/mixer units consists of either only endothermic units, interacting with a single hot reservoir, or only exothermic units interacting with a single cold reservoir, respectively⁵⁴. It has also been shown that when the universe of realizable reactor/mixer units consists of both endothermic and exothermic units, the network's entropy generation and energy consumption depend on the network structure⁵⁴. These results have provided the inspiration for the work presented in this manuscript. Indeed, close examination of the reactions taking place in a reformer reveals that the universe of realizable reformer units consists of both endothermic and exothermic units. In turn, this realization suggests that the energy consumption characteristics of an overall hydrogen production network (flowsheet) depend on the network structure, and can be dramatically altered, through the possible use of

endothermic and/or exothermic reformer units, thus opening up dramatic opportunities for process intensification according to the latter's expanded definition³³.

In this work, the IDEAS framework is employed for process flowsheet intensification. Process flowsheets are networks that employ a variety of process units, including reactors, separators, pumps, compressors, turbines, valves, heat exchangers, and many others. As stated earlier, one way to intensify a process is to increase the efficiency of its energy use. Thus, the process intensification goal that we aim to improve in this work will be the cost of the hot and cold utilities consumed by the process, which we will minimize. Hot and cold utilities at multiple temperature levels will be considered, reflecting the availability of both renewable and non-renewable energy resources. Possible opportunities for heat integration will also be explored by incorporating heat exchanger network (HEN) synthesis in the overall process network (PN) synthesis task, and carrying out simultaneously HEN and PN synthesis. Models for all the processes employed in this work are presented next, and the applicability of IDEAS to each such process model is ascertained. First however, Proposition 1 is proved, which is subsequently used to establish the applicability of IDEAS to the reactor model employed in this work. Proposition 1 provides a means of reducing the dimension of the state-space over which process intensification is pursued. The proposition allows for the scaling of the Gibbs free energy minimization problem, that determines the equilibrium reactor's exit compositions. Since the underlying objective function is a nonlinear homogenous function, a reduction in the dimensionality of the underlying state-space is achieved. For the considered case study, use of the equilibrium reactor models, combined with Proposition 1, enables the search for energy efficient designs to be carried out in the two-dimensional space of atomic fraction ratios, rather than the four-

dimensional-space of species (CH₄, CO, CO₂, H₂O) mole fractions (H₂ mole fraction is calculated in any case).

Proposition 1

Consider the following two optimization problems, where:

$$\left\{ \begin{array}{l} \nu(a) = f(\hat{n}) \triangleq \min_{n \in \mathbb{R}^k} f(n) \\ \text{s.t. } An = a \\ n \geq 0 \end{array} \right\} \text{ and } \left\{ \begin{array}{l} \nu(\lambda a) = f(\hat{n}_\lambda) \triangleq \min_{n_\lambda \in \mathbb{R}^k} f(n_\lambda) \\ \text{s.t. } An_\lambda = \lambda a \\ n_\lambda \geq 0 \end{array} \right\}$$

where $\lambda > 0$, $A \in \mathbb{R}^{l \times k}$, $a \in \mathbb{R}^l$ and $f(\cdot)$ is a homogeneous function of degree one, i.e.

$$f: \mathbb{R}^k \rightarrow \mathbb{R}, f: n \rightarrow f(n), f: \lambda n \rightarrow f(\lambda n) = \lambda f(n) \quad \forall \lambda > 0 \quad \forall n \in \mathbb{R}^k.$$

Then,

- $\nu(\lambda a) = f(\hat{n}_\lambda) = f(\lambda \hat{n}) = \lambda f(\hat{n}) = \lambda \nu(a).$
- If the optimization problem $\nu(a)$ has a unique global optimum $\forall a \in \mathbb{R}^l$, then

$$\hat{n}_\lambda = \lambda \hat{n} \quad \forall \lambda > 0.$$

Proof:

- Based on the proposition statement, $\hat{n}$ and $\hat{n}_\lambda$ are the global minima of $\nu(a)$ and $\nu(\lambda a)$ respectively.

Since $\left\{ \begin{array}{l} A\hat{n} = a \\ \hat{n} \geq 0 \end{array} \right\} \xLeftrightarrow{\lambda > 0} \left\{ \begin{array}{l} A\lambda\hat{n} = \lambda a \\ \lambda\hat{n} \geq 0 \end{array} \right\}$, then $\lambda\hat{n}$ is a feasible point of $\nu(\lambda a)$.

This means that $f(\lambda\hat{n}) \geq f(\hat{n}_\lambda) = \nu(\lambda a).$

Define $\bar{n}_\lambda \triangleq \frac{1}{\lambda} \hat{n}_\lambda$.

Since $\left\{ \begin{array}{l} A\hat{n}_\lambda = \lambda a \\ \hat{n}_\lambda \geq 0 \end{array} \right\} \xLeftrightarrow{\lambda > 0} \left\{ \begin{array}{l} \frac{1}{\lambda} A\hat{n}_\lambda = \frac{1}{\lambda} \lambda a \\ \frac{1}{\lambda} \hat{n}_\lambda \geq 0 \end{array} \right\} \xLeftrightarrow{\bar{n}_\lambda = \frac{1}{\lambda} \hat{n}_\lambda} \left\{ \begin{array}{l} A\bar{n}_\lambda = a \\ \bar{n}_\lambda \geq 0 \end{array} \right\}$, then, $\bar{n}_\lambda$ is a feasible point for $\nu(a)$.

This means that $f(\bar{n}_\lambda) \geq f(\hat{n}) = \nu(a)$.

In addition, since $f(\cdot)$ is a homogeneous function, it holds $f\left(\frac{1}{\lambda} \hat{n}_\lambda\right) = \frac{1}{\lambda} f(\hat{n}_\lambda)$.

It then holds,

$$\nu(a) = f(\hat{n}) \leq f(\bar{n}_\lambda) = f\left(\frac{1}{\lambda} \hat{n}_\lambda\right) = \frac{1}{\lambda} f(\hat{n}_\lambda) = \frac{1}{\lambda} \nu(\lambda a) \leq \frac{1}{\lambda} f(\lambda \hat{n}) = \frac{1}{\lambda} \lambda f(\hat{n}) = \nu(a). \text{O.E.}\Delta.$$

b. Consider, in addition that the optimization problem $\nu(a)$ has a unique global optimum

$$\forall a \in \mathbb{R}^l.$$

Let the global optimum of $\nu(\lambda a), \hat{n}_\lambda$, be such that $\hat{n}_\lambda \neq \lambda \hat{n}$. It holds however that $\lambda \hat{n}$ is a feasible point of $\nu(\lambda a)$. Then $f(\hat{n}_\lambda) < f(\lambda \hat{n})$, which in turn implies

$$\nu(\lambda a) = f(\hat{n}_\lambda) < f(\lambda \hat{n}) = \lambda f(\hat{n}) = \lambda \nu(a). \text{ This is in contradiction with } \nu(\lambda a) = \lambda \nu(a)$$

which was established in part a. above. Thus, $\hat{n}_\lambda = \lambda \hat{n}$. O.E.Δ.

Having established Proposition 1, we next outline the concept of a process information map and discuss how establishing a number of properties that process information maps naturally possess, enables the development of the IDEAS conceptual framework. Historically, in the modular approach to process simulation (see for example review⁴⁶) “each chemical

processing step is represented as a separate mathematical model called a unit module ... the process flow sheet is translated into an information flow sheet ... process topology may be expressed directly on the FORTRAN level by use of stream (information) vectors.” However, although information vectors were used to express process topology, information maps (and their properties) were not explicitly focused on. Process information maps taking inlet stream information (such as flows, component concentration, enthalpies, and so on) and transforming it to similar outlet stream information, give rise to process operators that are nonlinear, and result in nonconvex optimal network synthesis formulations. IDEAS provides a radical departure from this approach. IDEAS identifies input, and output vector decompositions and corresponding restricted input output information maps, so that three properties are satisfied, including linearity properties for these appropriately defined input output map restrictions. By then considering an infinite cardinality universe of units, it is able to fully account for chemical process nonlinearities prior to optimization, and only employ the aforementioned linear map restrictions during optimization. Indeed, IDEAS considers that the process operator OP takes extensive inlet stream information (e.g. total flow, component flows), available at an infinite collection of appropriately defined, fixed inlet conditions (e.g. temperature, concentration, residence time, etc.) and transforms it to extensive outlet stream information (e.g. total flow) available at the corresponding outlet conditions. The resulting IDEAS process operator is linear for any chemical process, as a result of the property of chemical processes, that when their inlet flow rates increase proportionally (without altering their associated inlet conditions), their outlet flow rates also increase by the same proportion, while their associated outlet conditions remain unaltered.

Thus, having established the linearity of the IDEAS process operator OP, we are now in a position to justify the claim that the IDEAS representation gives rise to linear problem

formulations. The constraints in the DN arise due to mixing and splitting operations, and are linear in the extensive (flow) variables. This fact, combined with the OP linearity, results in a linear feasible region that captures all possible process networks, by considering that the OP network inlets correspond to all possible associated conditions, and by allowing the DN network to consider all possible interconnections between external outlets (inlets)/OP inlets (outlets). In this work a novel reactor information map is provided, which utilizes a Gibbs free energy minimization model presented here for the first time for process synthesis purposes. Similarly, a novel separator information map is provided, which utilizes a minimum work of separation based model presented here for the first time for process synthesis purposes. Further, the stream creation process in the HEN operator, the mixing process preceding the distribution network, as well as the simultaneous synthesis of Heat Exchange Networks and Process Networks including Reactors and Separators, are all presented in this work for the first time. The applicability of IDEAS to all employed process models is accomplished by establishing that each process information map satisfies the following properties:

Consider the information map $\Psi : D_1 \times D_2 \subset \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \rightarrow \mathbb{R}^p$,

$$\Psi : u = \begin{bmatrix} u_1^T & | & u_2^T \end{bmatrix}^T \rightarrow \Psi(u) = \Psi(u_1, u_2)$$

that helps define the set D as follows: $D = \{u \in D_1 \times D_2 \subset \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} : \Psi(u_1, u_2) = 0\}$

Let the considered process model have information map $\Phi : D \subset \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \rightarrow \mathbb{R}^{m_1} \times \mathbb{R}^{m_2}$,

$$\Phi : u = \begin{bmatrix} u_1^T & | & u_2^T \end{bmatrix}^T \rightarrow y = \Phi(u) = \begin{bmatrix} y_1^T & | & y_2^T \end{bmatrix}^T = \begin{bmatrix} \left[\Phi_1(u_1, u_2) \right]^T & | & \left[\Phi_2(u_1, u_2) \right]^T \end{bmatrix}^T .$$

Having defined the maps Φ, Ψ , we can now state the properties that must hold to ensure IDEAS applicability.

Property 1:

$\exists \Psi_1 : \mathbb{R}^{n_1} \rightarrow \mathbb{R}^{p \times n_2}, \Psi_1 : u_1 \rightarrow \Psi_1(u_1)$ such that

$$\Psi(u_1, u_2) = \Psi_1(u_1)u_2 \quad \forall u = (u_1, u_2) \in D_1 \times D_2 \subset \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$$

Property 1 is best understood as follows: First, there exists a (possibly nonlinear) map (Ψ_1) that maps the unit sub-vector u_1 to a linear operator (matrix) $\Psi_1(u_1)$ that belongs to the space of matrices $\mathbb{R}^{p \times n_2}$. Then, the image of the vector (u_1, u_2) through the map Ψ is the composition of the linear operator $\Psi_1(u_1)$ with the sub-vector u_2 .

Property 2:

$\exists \Phi_3 : \mathbb{R}^{n_1} \rightarrow \mathbb{R}^{m_1}, \Phi_3 : u_1 \rightarrow \Phi_3(u_1)$ such that

$$y_1 = \Phi_1(u_1, u_2) = \Phi_3(u_1) \quad \forall u = (u_1, u_2) \in D \subset \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$$

Property 2 implies that $y_1 = \Phi_1(u_1, u_2)$ can be evaluated based only on knowledge of u_1 , without requiring any knowledge of u_2 .

Property 3:

$\exists \Phi_4 : \mathbb{R}^{n_1} \rightarrow \mathbb{R}^{m_2 \times n_2}, \Phi_4 : u_1 \rightarrow \Phi_4(u_1)$ such that

$$\Phi_2(u_1, u_2) = \Phi_4(u_1)u_2 \quad \forall u = (u_1, u_2) \in D \subset \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$$

Property 3 is best understood as follows: First, there exists a (possibly nonlinear) map (Φ_4) that maps the unit sub-vector u_1 to a linear operator (matrix) $\Phi_4(u_1)$ that belongs to the space of matrices $\mathbb{R}^{m_2 \times n_2}$. Then, the image of the vector (u_1, u_2) through the map Φ is the composition of the linear operator $\Phi_4(u_1)$ with the sub-vector u_2 .

A demonstration of these properties for a reactive distillation separator model is presented below for illustrative purposes. Let F^L , F^V , F^P be the liquid outlet, vapor outlet, and inlet total molar flows respectively. Let also f_i^P be the i th component's inlet molar flow rate, and x_i^L , y_i^V be the i th component's mole fractions of the liquid and vapor outlets respectively. Finally, let $R_i(\{x_j^L\}_1^{n-1})$ be the i th component's generation rate, P_i^{sat} , γ_i be the i th component's saturation pressure, and activity coefficient respectively, P be the total pressure, and H be the liquid molar holdup.

The corresponding IDEAS information map is then defined as follows:

$$\begin{aligned}
 u &= \begin{bmatrix} u_1^T & | & u_2^T \end{bmatrix}^T = \begin{bmatrix} x_1^L & \cdots & x_{n-1}^L & | & f_1^P & \cdots & f_n^P & F^L & F^V & H \end{bmatrix}^T \\
 y &= \begin{bmatrix} y_1^T & | & y_2^T \end{bmatrix}^T = \begin{bmatrix} x_1^L & \cdots & x_n^L & x_n^L & y_1^V & \cdots & y_n^V & | & f_1^P & \cdots & f_n^{in} & F^L & F^V & H & F^P \end{bmatrix}^T \\
 u_1 \in D_1 &\triangleq \left\{ u_1 = \begin{bmatrix} x_1^L & \cdots & x_{n-1}^L \end{bmatrix}^T \in \mathbb{R}^{n-1} : x_i^L \geq 0 \ \forall i = 1, n-1; 1 - \sum_{i=1}^{n-1} x_i^L \geq 0 \right\} \\
 u_2 \in D_2 &\triangleq \left\{ u_2 = \begin{bmatrix} f_1^P & \cdots & f_n^P & F^L & F^V & H \end{bmatrix}^T \in \mathbb{R}^{n+3} : \right. \\
 &\quad \left. F^L \geq 0, F^V \geq 0, H \geq 0, f_k^P \geq 0 \ \forall k = 1, n \right\}
 \end{aligned}$$

Property 1: the map $\Psi_1: \mathbb{R}^{n-1} \supset D_1 \rightarrow \mathbb{R}^{n \times (n+3)}$ for the considered model is defined as follows:

$$\Psi_1 : u_1 \triangleq \begin{bmatrix} x_1^L & \cdots & x_{n-1}^L \end{bmatrix} \rightarrow \Psi_1(u_1) \triangleq \begin{bmatrix} 1 & \cdots & 0 & -x_1^L & -y_1^V \left(\{x_k^L\}_1^{n-1} \right) & R_1 \left(\{x_k^L\}_1^{n-1} \right) \\ 0 & \ddots & 0 & \vdots & \vdots & \vdots \\ 0 & \cdots & 1 & -\left(1 - \sum_{i=1}^{n-1} x_i^L \right) & -y_n^L \left(\{x_k^L\}_1^{n-1} \right) & R_n \left(\{x_k^L\}_1^{n-1} \right) \end{bmatrix}^T,$$

$$\text{and } \Psi_1(u_1)u_2 = \begin{bmatrix} 1 & \cdots & 0 & -x_1^L & -y_1^V \left(\{x_k^L\}_1^{n-1} \right) & R_1 \left(\{x_k^L\}_1^{n-1} \right) \\ 0 & \ddots & 0 & \vdots & \vdots & \vdots \\ 0 & \cdots & 1 & -\left(1 - \sum_{i=1}^{n-1} x_i^L \right) & -y_n^L \left(\{x_k^L\}_1^{n-1} \right) & R_n \left(\{x_k^L\}_1^{n-1} \right) \end{bmatrix}^T \begin{bmatrix} f_1^P \\ \vdots \\ f_n^P \\ F^L \\ F^V \\ H \end{bmatrix} = 0$$

Property 2: the map $\Phi_3 : \mathbb{R}^{n-1} \supset D_1 \rightarrow \mathbb{R}^{2n}$ is defined as follows:

$$\Phi_3 : u_1 \rightarrow y_1 \triangleq \begin{bmatrix} x_1^L \\ \vdots \\ x_{n-1}^L \\ x_n^L \\ y_1^V \\ \vdots \\ y_n^V \end{bmatrix} = \Phi_3(u_1) \triangleq \begin{bmatrix} x_1^L \\ \vdots \\ x_{n-1}^L \\ 1 - \sum_{k=1}^{n-1} x_k^L \\ \frac{P_1^{sat} \gamma_1}{P} x_1^L \\ \vdots \\ \frac{P_n^{sat} \gamma_n}{P} x_n^L \end{bmatrix}$$

Property 3: the map $\Phi_4 : \mathbb{R}^{n-1} \supset D_1 \rightarrow \mathbb{R}^{(n+4) \times (n+3)}$ is defined as follows:

$$\Phi_4 : u_1 \rightarrow \Phi_4(u_1) \triangleq \begin{bmatrix} 1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 & 0 & 0 \\ 0 & \cdots & 1 & 0 & 0 & 0 \\ 0 & \cdots & 0 & 1 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 1 & 0 \\ 0 & \cdots & 0 & 0 & 0 & 1 \\ 1 & \cdots & 1 & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{(n+4) \times (n+3)}, \text{ and}$$

$$y_2 = \begin{bmatrix} f_1^P \\ \vdots \\ f_n^P \\ F^L \\ F^V \\ H \\ F^P \end{bmatrix} = \Phi_4(u_1) u_2 = \begin{bmatrix} 1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 & 0 & 0 \\ 0 & \cdots & 1 & 0 & 0 & 0 \\ 0 & \cdots & 0 & 1 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 1 & 0 \\ 0 & \cdots & 0 & 0 & 0 & 1 \\ 1 & \cdots & 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} f_1^P \\ \vdots \\ f_n^P \\ F^L \\ F^V \\ H \end{bmatrix}$$

Once these properties have been established, an infinite sequence $\{u_1(i)\}_{i=1}^{\infty}$ that consists of all possible values of u_1 such that the union of u_1 values considered is dense in the set where u_1 can vary, is considered. The sequences $\{\Psi_1(u_1(i))\}_{i=1}^{\infty}, \{\Phi_4(u_1(i))\}_{i=1}^{\infty}, \{\Phi_3(u_1(i))\}_{i=1}^{\infty}$ of linear maps and vectors belonging to $\mathbb{R}^{p \times n_2}, \mathbb{R}^{m_2 \times n_2}, \mathbb{R}^{m_1}$ respectively can then be created using the maps Ψ_1, Φ_4, Φ_3 respectively. These sequences can then be used to evaluate the infinite sequence of domains for $\{u_2(i)\}_{i=1}^{\infty}$, the infinite sequence $\{y_2(i)\}_{i=1}^{\infty} = \{\Phi_4(u_1(i)) \cdot u_2(i)\}_{i=1}^{\infty}$ and the infinite sequence $\{y_1(i)\}_{i=1}^{\infty} = \{\Phi_3(u_1(i))\}_{i=1}^{\infty}$.

Next, utilizing these three properties the applicability of IDEAS is established for all unit operations considered in this work.

Reactors

For the considered case study, use of equilibrium reactor models is considered, since it is well known that industrial reformers operate near equilibrium (see reference 55). In addition, the use of equilibrium reactor models, combined with Proposition 1, enables the search for energy efficient designs to be carried out in the space of atomic fraction ratios, rather than the space of species mole fractions. In particular, a Gibbs free energy minimization problem is solved to identify the reactor's exit species concentrations using only temperature, pressure, and inlet atomic ratio specifications. The indices $i = 1, m ; j = 1, n ; k = 1, NP$ denote the i th atom, j th species, and k th phase respectively, and the variables α, n, T, P, G denote the atomic mass flow rate (kg/s), molar flow rate (moles/s), temperature (K), pressure (bar), and Gibbs free energy (kJ) respectively. The indices NC, NE, NP are the number of components, the number of elements, and the number of phases respectively, and the variables $\mu, \nu_{i,j}$ denote the chemical potential (J/mol), the number of i th type atoms in the j th species' molecule.

$$\left\{ \begin{array}{l} \pi(T, P, \{\alpha_i\}_{i=1}^m) \triangleq \min_{\substack{\{n_j^{(k)}\}_{(j,k)=(1,1)}^{(NC,NP)}}} G\left(T, P, \{n_p^{(k)}\}_{(p,k)=(1,1)}^{(n,NP)}\right) \\ s.t. \quad \alpha_i - \sum_k^{NP} \sum_j^n M_i \nu_{ij} n_j^{(k)} = 0 \quad \forall i = 1, NE \\ \quad \quad n_j^{(k)} \geq 0 \quad \forall j = 1, NC; \quad \forall k = 1, NP \end{array} \right\}, \text{ where}$$

$$G\left(T, P, \{n_p^{(k)}\}_{(p,k)=(1,1)}^{(n,NP)}\right) = \sum_{k=1}^{NP} \sum_{j=1}^n n_j^{(k)} \mu_j^{(k)} \left(T, P, \left\{ \frac{n_j^{(k)}}{\sum_{l=1}^n n_l^{(k)}} \right\}_{j=1}^n \right). \text{ Application of the aforementioned}$$

proposition 1 to this optimization problem necessitates that the objective function be first order

homogeneous. In general, $G\left(T, P, \{n_p^{(k)}\}_{(p,k)=(1,1)}^{(n,NP)}\right)$ is a function of $n \times NP + 2$ variables, and when

treated as such it is not homogeneous. However, when T, P are fixed at $T = \bar{T}, P = \bar{P}$, then the

restriction of G at $T = \bar{T}, P = \bar{P}, G\left(\bar{T}, \bar{P}, \left\{n_p^{(k)}\right\}_{(p,k)=(1,1)}^{(n, NP)}\right)$, is a first order homogenous function.

Indeed, let $\lambda > 0$. Then

$$G\left(\bar{T}, \bar{P}, \left\{\lambda n_p^{(k)}\right\}_{(p,k)=(1,1)}^{(n, NP)}\right) = \sum_{k=1}^{NP} \sum_{j=1}^n \lambda n_j^{(k)} \mu_j^{(k)} \left(T, P, \left\{ \frac{\lambda n_j^{(k)}}{\sum_{l=1}^n \lambda n_l^{(k)}} \right\}_{j=1}^n \right) \Leftrightarrow$$

$$G\left(\bar{T}, \bar{P}, \left\{\lambda n_p^{(k)}\right\}_{(p,k)=(1,1)}^{(n, NP)}\right) = \lambda \left\{ \sum_{k=1}^{NP} \sum_{j=1}^n n_j^{(k)} \mu_j^{(k)} \left(T, P, \left\{ \frac{n_j^{(k)}}{\sum_{l=1}^n n_l^{(k)}} \right\}_{j=1}^n \right) \right\} \Leftrightarrow$$

$$G\left(\bar{T}, \bar{P}, \left\{\lambda n_p^{(k)}\right\}_{(p,k)=(1,1)}^{(n, NP)}\right) = \lambda G\left(\bar{T}, \bar{P}, \left\{n_p^{(k)}\right\}_{(p,k)=(1,1)}^{(n, NP)}\right)$$

Since $G\left(\bar{T}, \bar{P}, \left\{n_p^{(k)}\right\}_{(p,k)=(1,1)}^{(n, NP)}\right)$ is a first order homogenous function, the problem constraints are

linear, and the problem variables are nonnegative, and proposition 1 can be applied. Selecting

$\lambda \triangleq 1 / \sum_i^m \alpha_i > 0$, then yields:

$$\left\{ \begin{array}{l} \pi \left(T, P, \left\{ \frac{\alpha_i}{\sum_i \alpha_i} \right\}_{i=1}^m \right) \hat{=} \min_{\left\{ \frac{n_j^{(k)}}{\sum_i \alpha_i} \right\}_{(j,k)=(1,1)}^{(n, NP)}} G \left(T, P, \left\{ \frac{n_p^{(k)}}{\sum_i \alpha_i} \right\}_{(p,k)=(1,1)}^{(n, NP)} \right) \\ s.t. \quad \frac{\alpha_i}{\sum_i \alpha_i} - \sum_k^{NP} \sum_j^n M_i v_{ij} \frac{n_j^{(k)}}{\sum_i \alpha_i} = 0 \quad \forall i = 1, m \\ \frac{n_j^{(k)}}{\sum_i \alpha_i} \geq 0 \quad \forall j = 1, n; \quad \forall k = 1, NP \end{array} \right\}$$

where $\frac{\alpha_i}{\sum_i \alpha_i}$ is the mass fraction of the i th element.

It is this optimization that will be solved to model the reactor units in this work.

The IDEAS information maps for reactors are then defined as follows. Let T^V , P^V , P^W be the outlet temperature (K), outlet pressure (bar), and inlet pressure (bar) respectively. Let also,

$\left\{ \frac{\alpha_i^W}{\sum_i \alpha_i^W} \right\}_{i=1}^m$ be the atomic mass fraction of the i th species, and $\{x_k^V\}_{k=1}^n$ the mass fraction of the

unit's outlet k th species. Finally, let h^V , H^W , $\dot{Q}$ be the outlet stream's specific enthalpy (kJ/kg), inlet stream's heat flow (kJ/s), and unit's heat load respectively (kJ/s), and F^W , F^V , f_k^W be the unit's inlet flow rate (kg/s), unit's outlet flow rate (kg/s), and unit inlet's k th species mass flow rate (kg/s). The subscript PR represents the Peng-Robinson equation of state model.

$$u = \begin{bmatrix} u_1^T & | & u_2^T \end{bmatrix}^T = \begin{bmatrix} T^V & P^V & \left\{ \frac{\alpha_i^W}{\sum_{i=1}^m \alpha_i^W} \right\}^m & | & F^W & f_1^W & \dots & f_n^W & \dot{Q} \end{bmatrix}^T$$

$$y = \begin{bmatrix} y_1^T & | & y_2^T \end{bmatrix}^T = \begin{bmatrix} T^V & P^V & \left\{ \frac{\alpha_i^W}{\sum_{i=1}^m \alpha_i^W} \right\}^m & P^W & \{x_k^V\}_{k=1}^n & h^V & | & F^W & \dot{Q} & f_1^W & \dots & f_2^W & F^V & H^W \end{bmatrix}^T$$

$$\text{where } u_1 \in D_1 \triangleq \left\{ \begin{array}{l} u_1 = \begin{bmatrix} T^V & P^V & \left\{ \frac{\alpha_i^W}{\sum_{i=1}^m \alpha_i^W} \right\}^m \end{bmatrix}^T \in \mathbb{R}^{m+2} : \\ T^V \geq 0, P^V \geq 0, \sum_{i=1}^m \frac{\alpha_i^W}{\sum_{i=1}^m \alpha_i^W} = 1, \frac{\alpha_i^W}{\sum_{i=1}^m \alpha_i^W} \geq 0 \quad \forall i = 1, m \end{array} \right\}$$

$$u_2 \in D_2 \triangleq \left\{ \begin{array}{l} u_2 = \begin{bmatrix} F^W & f_1^W & \dots & f_n^W & \dot{Q} \end{bmatrix}^T \in \mathbb{R}^{n+2} : F^W \geq 0, f_k^W \geq 0 \quad \forall k = 1, n \\ \left\{ \begin{array}{l} \dot{Q} \geq 0 \text{ if reactor is heated} \\ \dot{Q} \leq 0 \text{ if reactor is cooled} \end{array} \right\} \end{array} \right\}$$

The map $\Psi_1 : \mathbb{R}^{m+2} \supset D_1 \rightarrow \mathbb{R}^{m \times (n+2)}$ for the considered reactor model is defined as follows:

$$\Psi_1 : u_1 \rightarrow \Psi_1(u_1) \triangleq \begin{bmatrix} \frac{\alpha_1^W}{\sum_i^m \alpha_i^W} & -R_{1,1}^W & \cdots & -R_{1,n}^W & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\alpha_m^W}{\sum_i^m \alpha_i^W} & -R_{m,1}^W & \cdots & -R_{m,n}^W & 0 \end{bmatrix}^T \in \mathbb{R}^{m \times (n+2)}, \text{ and}$$

$$\Psi_1(u_1)u_2 = \begin{bmatrix} \frac{\alpha_1^W}{\sum_i^m \alpha_i^W} & -R_{1,1}^W & \cdots & -R_{1,n}^W & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\alpha_m^W}{\sum_i^m \alpha_i^W} & -R_{m,1}^W & \cdots & -R_{m,n}^W & 0 \end{bmatrix}^T \begin{bmatrix} F^W \\ f_1^W \\ \vdots \\ f_n^W \\ \dot{Q} \end{bmatrix} = 0$$

Where $R_{i,k}^W = (ANM^{-1})_{i,k}$, $i = 1, m$; $k = 1, n$, where A is the diagonal matrix, $A = \begin{bmatrix} A_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & A_m \end{bmatrix}$,

whose entries are the molar masses of each atom or each inert molecule, N is the matrix,

$$N = \begin{bmatrix} \nu_{1,1} & \cdots & \nu_{1,n} \\ \vdots & \ddots & \vdots \\ \nu_{m,1} & \cdots & \nu_{m,n} \end{bmatrix}, \text{ of stoichiometric coefficients, } \nu_{i,k} \text{ that quantify the number of } i\text{th atoms}$$

in the k th species, and M is the diagonal matrix, $M = \begin{bmatrix} M_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & M_n \end{bmatrix}$, whose entries are the

molar masses of each species.

The maps $\Phi_3 : \mathbb{R}^{m+2} \supset D_1 \rightarrow \mathbb{R}^{m+n+4}$ and $\Phi_4 : \mathbb{R}^{m+2} \supset D_1 \rightarrow \mathbb{R}^{(n+4) \times (n+2)}$ are defined as follows:

$$\Phi_3 : u_1 \rightarrow y_1 = \Phi_3(u_1) \triangleq \begin{bmatrix} T^V \\ P^V \\ \left\{ \frac{\alpha_i^W}{\sum_i^m \alpha_i^W} \right\}_{i=1}^m \\ P^V \\ \left\{ M_k \cdot \arg \min \pi \left(T^V, P^V, \left\{ \frac{\alpha_i^W}{\sum_i^m \alpha_i^W} \right\}_{i=1}^m \right) \right\}_{k=1}^n \\ h_{PR} \left(T^V, P^V, \left\{ M_k \cdot \arg \min \pi \left(T^V, P^V, \left\{ \frac{\alpha_i^W}{\sum_i^m \alpha_i^W} \right\}_{i=1}^m \right) \right\}_{k=1}^n \right) \end{bmatrix}$$

$$\Phi_4 : u_1 \rightarrow \Phi_4(u_1) \triangleq \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ h^V & 0 & 0 & 0 & 1 \end{bmatrix} \in \mathbb{R}^{(n+4) \times (n+2)}, \text{ and}$$

$$y_2 = \begin{bmatrix} F^W \\ \dot{Q} \\ f_1^W \\ \vdots \\ f_n^W \\ F^V \\ H^W \end{bmatrix} = \Phi_4(u_1)u_2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ h^V & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} F^W \\ f_1^W \\ \vdots \\ f_n^W \\ \dot{Q} \end{bmatrix}$$

Separators

As can be seen in Figure 1, heat is only allowed to leave the separator at a temperature T , enter an ideal Carnot Cycle, which releases heat to the environment, and generates some work which enters the separator. That work, combined with additional work that enters the separator, so as to satisfy its energetic needs

Figure 1: Separator Representation

for separation, allows computation of the ideal work of separation. This separator type is similar to the separators used for the gas separation tasks typical of the considered case study (membrane separators, pressure swing adsorbers, etc.)

The considered separator model is assumed to have no heat inlet ports, a single heat outlet port at a temperature T above the environmental temperature T_σ , and inlet and outlet streams with potential and kinetic energy terms that can be neglected. A Carnot engine is coupled to separator units, so as to calculate the ideal work of separation, which is later used in the IDEAS formulation for the separator units. Consider also that the separator is coupled to a power engine operating between T and T_σ . Then, the following proposition holds:

Proposition 2

Consider a separator operating at steady-state, having a single outlet heat port at $T \geq T_\sigma$, and inlet and outlet streams with potential, and kinetic energy terms that can be neglected. Let H denote the enthalpy of a stream, S denote the entropy of a stream, S_O denote the index set of the

outlet streams, and S_i denote the index set of the inlet streams. Then the ideal work of separation, and the associated ideal separator cold utility load are:

$$\dot{W} = \sum_{i \in S_O} F_i (H_i - T_\sigma S_i) - \sum_{i \in S_I} F_i (H_i - T_\sigma S_i)$$

$$\dot{Q}_\sigma = \sum_{i \in S_I} F_i T_\sigma S_i - \sum_{i \in S_O} F_i T_\sigma S_i.$$

Proof:

$$\left\{ \begin{array}{l} 0 = \sum_{i \in S_I} F_i H_i - \sum_{i \in S_O} F_i H_i - \dot{Q} + \dot{W} + \dot{W}_\sigma \\ 0 = \sum_{i \in S_I} F_i S_i - \sum_{i \in S_O} F_i S_i - \frac{\dot{Q}}{T} + \dot{S}_G \wedge \dot{S}_G \geq 0 \\ 0 = \dot{Q} - \dot{Q}_\sigma - \dot{W}_\sigma \\ 0 = \frac{\dot{Q}}{T} - \frac{\dot{Q}_\sigma}{T_\sigma} + \dot{S}_{G,\sigma} \wedge \dot{S}_{G,\sigma} \geq 0 \end{array} \right\} \Leftrightarrow \left\{ \begin{array}{l} \dot{W} + \dot{W}_\sigma = - \sum_{i \in S_I} F_i H_i + \sum_{i \in S_O} F_i H_i + \dot{Q} \\ \dot{Q} = T \sum_{i \in S_I} F_i S_i - T \sum_{i \in S_O} F_i S_i + T \dot{S}_G \wedge \dot{S}_G \geq 0 \\ \dot{W}_\sigma = \left(1 - \frac{T_\sigma}{T}\right) \dot{Q} - T_\sigma \dot{S}_{G,\sigma} \\ \dot{Q}_\sigma = \frac{T_\sigma}{T} \dot{Q} + T_\sigma \dot{S}_{G,\sigma} \wedge \dot{S}_{G,\sigma} \geq 0 \end{array} \right\} \Leftrightarrow$$

$$\left\{ \begin{array}{l} \dot{W} + \dot{W}_\sigma = \sum_{i \in S_O} F_i (H_i - T S_i) - \sum_{i \in S_I} F_i (H_i - T S_i) + T \dot{S}_G \\ \dot{Q} = T \sum_{i \in S_I} F_i S_i - T \sum_{i \in S_O} F_i S_i + T \dot{S}_G \wedge \dot{S}_G \geq 0 \\ \dot{W}_\sigma = (T - T_\sigma) \left(\sum_{i \in S_I} F_i S_i - \sum_{i \in S_O} F_i S_i + \dot{S}_G \right) - T_\sigma \dot{S}_{G,\sigma} \\ \dot{Q}_\sigma = T_\sigma \left(\sum_{i \in S_I} F_i S_i - \sum_{i \in S_O} F_i S_i + \dot{S}_G \right) + T_\sigma \dot{S}_{G,\sigma} \wedge \dot{S}_{G,\sigma} \geq 0 \end{array} \right\} \Leftrightarrow$$

$$\left\{ \begin{array}{l} \dot{W} = \sum_{i \in S_O} F_i (H_i - T_\sigma S_i) - \sum_{i \in S_I} F_i (H_i - T_\sigma S_i) + T_\sigma (\dot{S}_G + \dot{S}_{G,\sigma}) \\ \dot{Q} = T \sum_{i \in S_I} F_i S_i - T \sum_{i \in S_O} F_i S_i + T \dot{S}_G \wedge \dot{S}_G \geq 0 \\ \dot{W}_\sigma = (T - T_\sigma) \left(\sum_{i \in S_I} F_i S_i - \sum_{i \in S_O} F_i S_i + \dot{S}_G \right) - T_\sigma \dot{S}_{G,\sigma} \\ \dot{Q}_\sigma = \sum_{i \in S_I} F_i T_\sigma S_i - \sum_{i \in S_O} F_i T_\sigma S_i + T_\sigma (\dot{S}_G + \dot{S}_{G,\sigma}) \wedge \dot{S}_{G,\sigma} \geq 0 \wedge \dot{S}_G \geq 0 \end{array} \right\}$$

The ideal work of separation is obtained by considering that the separator, and the coupled power engine are both reversible (their rates of entropy generation are both zero), i.e. $\dot{S}_G = 0 \wedge \dot{S}_{G,\sigma} = 0$.

Then the ideal work of separation, and the associated ideal separator cold utility load are:

$$\dot{W}_{Ideal} = \sum_{i \in S_O} F_i (H_i - T_\sigma S_i) - \sum_{i \in S_I} F_i (H_i - T_\sigma S_i)$$

$$\dot{Q}_{\sigma, Ideal} = \sum_{i \in S_I} F_i T_\sigma S_i - \sum_{i \in S_O} F_i T_\sigma S_i \cdot \text{O.E.}\Delta.$$

The IDEAS information maps for separators are then defined as follows. Let T_i^V, T^W, P_i^V, P^W be the unit's i th outlet temperature (K), unit's inlet temperature (K), unit's i th outlet pressure (bar), and unit's inlet pressure (bar) respectively. Let also $\{x_k^V\}_{k=1}^n$ be the mass fraction of the unit's outlet k th species, and h_i^V, H^W, s_i^V, S^W be the i th outlet stream's specific enthalpy (kJ/kg), inlet stream's heat flow (kJ/s), unit's i th outlet specific entropy (kJ/kg K), and inlet entropy flow of the stream (kJ/s K) respectively. Finally, let F^W, f_k^W, F_i^V be the unit's inlet flow rate (kg/s), i th unit's outlet flow rate (kg/s), and unit inlet's k th species mass flow rate (kg/s) respectively, and $\dot{Q}, \dot{W}_{Ideal}$ be the reactor's heat load (kJ/s) and ideal work (kJ/s) respectively. The subscript PR represents the Peng-Robinson equation of state model.

$$\begin{aligned} u &= \begin{bmatrix} u_1^T & | & u_2^T \end{bmatrix}^T = \begin{bmatrix} T_1^V & P_1^V & \{x_{1,k}^V\}_{k=1}^n & \{x_{2,k}^V\}_{k=1}^n & | & F_1^V & F_2^V & H^W & S^W \end{bmatrix}^T \\ y &= \begin{bmatrix} y_1^T & | & y_2^T \end{bmatrix}^T ; \\ y_1 &= \begin{bmatrix} T_1^V & P_1^V & \{x_{1,k}^V\}_{k=1}^n & \{x_{2,k}^V\}_{k=1}^n & T_2^V & T^W & P_2^V & P^W & h_1^V & h_2^V & s_1^V & s_2^V \end{bmatrix}^T \\ y_2 &= \begin{bmatrix} F_1^V & F_2^V & f_1^W & \dots & f_n^W & H^W & S^W & F^W & \dot{Q} & \dot{W}_{Ideal} \end{bmatrix}^T \end{aligned}$$

$$\text{where } u_1 \in D_1 = \left\{ u_1 = \begin{bmatrix} T_1^V & P_1^V & \{x_{1,k}^V\}_{k=1}^n & \{x_{2,k}^V\}_{k=1}^n \end{bmatrix}^T \in \mathbb{R}^{2n+2} : \right. \\ \left. \begin{aligned} & T_1^V \geq 0, P_1^V \geq 0, \sum_{k=1}^n x_{1,k}^V = 1, x_{1,k}^V \geq 0, \forall k=1, n \\ & \sum_{k=1}^n x_{2,k}^V = 1, x_{2,k}^V \geq 0 \quad \forall k=1, n \end{aligned} \right\}$$

$$u_2 \in D_2 \triangleq \left\{ u_2 = \begin{bmatrix} F_1^V & F_2^V & H^W & S^W \end{bmatrix}^T \in \mathbb{R}^4 : F_1^V \geq 0, F_2^V \geq 0 \right\}$$

No map Ψ_1 need be defined for the considered separator model.

The maps $\Phi_3 : \mathbb{R}^{2n+2} \supset D_1 \rightarrow \mathbb{R}^{2n+10}$ and $\Phi_4 : \mathbb{R}^{2n+2} \supset D_1 \rightarrow \mathbb{R}^{(n+7) \times 4}$ are defined as follows:

$$\Phi_3 : u_1 \rightarrow y_1 = \Phi_3(u_1) \triangleq \begin{bmatrix} T_1^V \\ P_1^V \\ \{x_{1,k}^V\}_{k=1}^n \\ \{x_{2,k}^V\}_{k=1}^n \\ T_1^V \\ T_1^V \\ P_1^V \\ P_1^V \\ h_{PR} \left(T_1^V, P_1^V, \{x_{1,k}^V\}_{k=1}^n \right) \\ h_{PR} \left(T_1^V, P_1^V, \{x_{2,k}^V\}_{k=1}^n \right) \\ s_{PR} \left(T_1^V, P_1^V, \{x_{1,k}^V\}_{k=1}^n \right) \\ s_{PR} \left(T_1^V, P_1^V, \{x_{2,k}^V\}_{k=1}^n \right) \end{bmatrix} \in \mathbb{R}^{2n+10},$$

$$\Phi_4 : u_1 \rightarrow \Phi_4(u_1) \triangleq \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ x_{1,1}^V & x_{2,1}^V & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ x_{1,n}^V & x_{2,n}^V & 0 & 0 \\ 1 & 1 & 0 & 0 \\ -T_\sigma s_1^V & -T_\sigma s_2^V & 0 & T_\sigma \\ h_1^V - T_\sigma s_1^V & h_2^V - T_\sigma s_2^V & -1 & T_\sigma \end{bmatrix} \in \mathbb{R}^{(n+7) \times 4}, \text{ and}$$

$$y_2 = \begin{bmatrix} F_1^V \\ F_2^V \\ H^W \\ S^W \\ f_1^W \\ \vdots \\ f_n^W \\ F^W \\ \dot{Q} \\ W \end{bmatrix} = \Phi_4(u_1)u_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ x_{1,1}^V & x_{2,1}^V & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ x_{1,n}^V & x_{2,n}^V & 0 & 0 \\ 1 & 1 & 0 & 0 \\ -T_\sigma s_1^V & -T_\sigma s_2^V & 0 & T_\sigma \\ h_1^V - T_\sigma s_1^V & h_2^V - T_\sigma s_2^V & -1 & T_\sigma \end{bmatrix} \begin{bmatrix} F_1^V \\ F_2^V \\ H^W \\ S^W \end{bmatrix}$$

Pressure Changing Devices

The IDEAS information maps for pressure changing devices are then defined as follows. Let T^V ,

$T_{isentropic}^V, T^W, P^V, P^W$ be the outlet temperature (K), isentropic outlet temperature (K), inlet

temperature (K), outlet pressure (bar), and inlet pressure (bar) respectively. Let also $\{x_k^V\}_{k=1}^n$,

$\{x_k^W\}_{k=1}^n$ be the mass fraction of the unit's outlet kth species, and mass fraction of the unit's inlet

kth species respectively, and h^V, H^W be the outlet stream's specific enthalpy (kJ/kg), and inlet

stream's heat flow (kJ/s) respectively. Finally, let F^W, F^V be the unit's inlet flow rate (kg/s), and

unit's outlet flow rate (kg/s) respectively, and η the isentropic efficiency. The subscript PR represents the Peng-Robinson equation of state model.

$$u = \begin{bmatrix} u_1^T & | & u_2^T \end{bmatrix}^T = \begin{bmatrix} T^W & P^W & P^V & \{x_k^W\}_{k=1}^n & \zeta & | & F^W \end{bmatrix}^T$$

$$y = \begin{bmatrix} y_1^T & | & y_2^T \end{bmatrix}^T = \begin{bmatrix} T^W & P^W & P^V & \{x_k^W\}_{k=1}^n & \zeta & \{x_k^V\}_{k=1}^n & h^W & s^W & T_{isentropic}^V & T^V & h^V & | & F^W & F^V & f_1^W & \dots & f_n^W & H^W & W \end{bmatrix}^T$$

$$\text{where, } \zeta = \begin{cases} 1/\eta & \text{compressors / pumps} \\ \eta & \text{turbines} \\ 0 & \text{valves} \end{cases},$$

$$u_1 \in D_1 = \left\{ u_1 = \begin{bmatrix} T^W & P^W & P^V & \{x_k^W\}_{k=1}^n & \zeta \end{bmatrix}^T \in \mathbb{R}^{n+4} : \right. \\ \left. T^W \geq 0, P^W \geq 0, \sum_{k=1}^n x_k^W = 1, x_k^W \geq 0 \ \forall k = 1, n; 0 \leq \zeta \leq 1 \right\},$$

$$u_2 \in D_2 \triangleq \left\{ u_2 = \begin{bmatrix} F^W \end{bmatrix}^T \in \mathbb{R} : F^W \geq 0 \right\}$$

No map Ψ_1 need be defined for the considered pressure changing device model.

The maps $\Phi_3 : \mathbb{R}^{n+4} \supset D_1 \rightarrow \mathbb{R}^{2n+9}$ and $\Phi_4 : \mathbb{R}^{n+4} \supset D_1 \rightarrow \mathbb{R}^{(n+4) \times 1}$ are defined as follows:

$$\begin{aligned}
\Phi_3 : u_1 \rightarrow y_1 = \Phi_3(u_1) \triangleq & \begin{bmatrix} T^W \\ P^W \\ P^V \\ \{x_k^W\}_{k=1}^n \\ \zeta \\ \{x_k^W\}_{k=1}^n \\ h_{PR}\left(T^W, P^W, \{x_k^W\}_{k=1}^n\right) \\ s_{PR}\left(T^W, P^W, \{x_k^W\}_{k=1}^n\right) \\ T_{PR}\left(s_{PR}\left(T^W, P^W, \{x_k^W\}_{k=1}^n\right), P^V, \{x_k^W\}_{k=1}^n\right) \\ T_{PR}\left[\begin{bmatrix} \zeta h_{PR}\left(T_{PR}\left(s_{PR}\left(T^W, P^W, \{x_k^W\}_{k=1}^n\right), P^V, \{x_k^W\}_{k=1}^n\right), P^V, \{x_k^W\}_{k=1}^n\right) \\ h_{PR}\left(T^W, P^W, \{x_k^W\}_{k=1}^n\right)(1-\zeta) \end{bmatrix} + P^V, \{x_k^W\}_{k=1}^n\right) \\ \left[\begin{bmatrix} \zeta h_{PR}\left(T_{PR}\left(s_{PR}\left(T^W, P^W, \{x_k^W\}_{k=1}^n\right), P^V, \{x_k^W\}_{k=1}^n\right), P^V, \{x_k^W\}_{k=1}^n\right) \\ h_{PR}\left(T^W, P^W, \{x_k^W\}_{k=1}^n\right)(1-\zeta) \end{bmatrix} + \right] \end{bmatrix}
\end{aligned}$$

$$\begin{aligned}
\Phi_4 : u_1 \rightarrow \Phi_4(u_1) \triangleq & \begin{bmatrix} 1 \\ 1 \\ x_1^W \\ \vdots \\ x_n^W \\ h^W \\ \zeta \left[\begin{bmatrix} h_{PR}\left(T_{PR}\left(s_{PR}\left(T^W, P^W, \{x_k^W\}_{k=1}^n\right), P^V, \{x_k^W\}_{k=1}^n\right), P^V, \{x_k^W\}_{k=1}^n\right) \\ h_{PR}\left(T^W, P^W, \{x_k^W\}_{k=1}^n\right) \end{bmatrix} - \right] \end{bmatrix} \in \mathbb{R}^{(n+4) \times 1}
\end{aligned}$$

$$y_2 = \begin{bmatrix} F^W \\ F^V \\ f_1^W \\ \vdots \\ f_n^W \\ H^W \\ W \end{bmatrix} = \Phi_4(u_1)u_2 = \begin{bmatrix} 1 \\ 1 \\ x_1^W \\ \vdots \\ x_n^W \\ h^W \\ \zeta \begin{pmatrix} h_{PR} \left(T_{PR} \left(s_{PR} \left(T^W, P^W, \{x_k^W\}_{k=1}^n \right), P^V, \{x_k^W\}_{k=1}^n \right) \right) \\ P^V, \{x_k^W\}_{k=1}^n \\ -h_{PR} \left(T^W, P^W, \{x_k^W\}_{k=1}^n \right) \end{pmatrix} \end{bmatrix} \begin{bmatrix} F^W \end{bmatrix}$$

Heat Exchange Network

In this work, the heat exchanger network shown in Figure 2 is considered. It contains three categories of heat exchangers: hot stream - cold stream heat exchangers; stream - point load heat exchangers, where a stream is cooled (heated) by a cold (hot) point load; and point load -

Figure 2 Representation of heat exchange network structure

point load heat exchangers where hot (cold) point loads and cold (hot) point loads are matched. External utilities as well as unit loads are typically considered as either hot or cold point loads. Streams are created by comparing each state with every other state, for equality of the two states' pressure and composition components. Once all streams have been created, all feasible/desirable/non-forbidden stream-stream heat exchangers, stream-point load heat exchangers, and point load-point load heat exchangers are generated. Thermodynamic feasibility of each exchanger is verified throughout its length. The objective function to be minimized in this work is the overall utility cost, for all external hot utilities.

The IDEAS information maps for stream-stream heat exchangers, whose first stream is considered to be hot, are then defined as follows. Let $T_i^V, T_i^W, P_i^V, P_i^W$ be the unit's i th outlet temperature (K), unit's i th inlet temperature (K), unit's i th outlet pressure (bar), and unit's i th inlet pressure (bar) respectively, and $\{x_{i,k}^V\}_{k=1}^n, \{x_{i,k}^W\}_{k=1}^n$ be the mass fraction of the unit's i th outlet k th species and mass fraction of the unit's i th inlet k th species respectively. Let also h_i^V, h_i^W be the i th outlet stream's specific enthalpy (kJ/kg), and i th inlet stream's heat flow (kJ/s) respectively (the subscript PR represents the Peng-Robinson equation of state model). Finally, let F_i^W, F_i^V be the i th unit's inlet flow rate (kg/s), and i th unit's outlet flow rate (kg/s) respectively, and $\dot{Q}$ be the unit's heat load (kJ/s).

$$u = \begin{bmatrix} u_1^T & | & u_2^T \end{bmatrix}^T = \begin{bmatrix} T_1^V & T_2^V & T_1^W & T_2^W & P_1^V & P_2^V & \{x_{1,k}^V\}_{k=1}^n & \{x_{2,k}^V\}_{k=1}^n & | & F_1^W & F_2^W \end{bmatrix}^T$$

$$\left\{ y = \begin{bmatrix} y_1^T & | & y_2^T \end{bmatrix}^T = \begin{bmatrix} T_1^V & T_2^V & T_1^W & T_2^W & P_1^V & P_2^V & \{x_{1,k}^V\}_{k=1}^n & \{x_{2,k}^V\}_{k=1}^n & P_1^W & P_2^W & \{x_{1,k}^W\}_{k=1}^n & \{x_{2,k}^W\}_{k=1}^n & h_1^W & h_2^W & h_1^V & h_2^V & | & F_1^W & F_2^W & F_1^V & F_2^V & \dot{Q} \end{bmatrix}^T \right\}$$

$$\text{where } u_1 \in D_1 = \left\{ \begin{array}{l} u_1 = \begin{bmatrix} T_1^V & T_2^V & T_1^W & T_2^W & P_1^V & P_2^V & \{x_{1,k}^V\}_{k=1}^n & \{x_{2,k}^V\}_{k=1}^n \end{bmatrix}^T \in \mathbb{R}^{2n+6} : \\ T_1^V \geq 0, T_2^V \geq 0, T_1^W \geq 0, T_2^W \geq 0, P_1^V \geq 0, P_2^V \geq 0, \\ \sum_{k=1}^n x_{1,k}^V = 1, x_{1,k}^V \geq 0 \quad \forall k = 1, n; \sum_{k=1}^n x_{2,k}^V = 1, x_{2,k}^V \geq 0 \quad \forall k = 1, n \end{array} \right\}$$

$$u_2 \in D_2 \triangleq \left\{ u_2 = \begin{bmatrix} F_1^W & F_2^W \end{bmatrix}^T \in \mathbb{R}^2 : F_1^W \geq 0, F_2^W \geq 0 \right\}$$

The map $\Psi_1 : \mathbb{R}^{2n+6} \supset D_1 \rightarrow \mathbb{R}^{1 \times 2}$ for the considered stream-stream heat exchanger model is defined as follows:

$$\Psi_1 : u_1 \rightarrow \Psi_1(u_1) \triangleq \begin{bmatrix} h_1^W - h_1^V & h_2^W - h_2^V \end{bmatrix} \in \mathbb{R}^{1 \times 2}, \text{ and } \Psi_1(u_1)u_2 = \begin{bmatrix} h_1^W - h_1^V & h_2^W - h_2^V \end{bmatrix} \begin{bmatrix} F_1^V \\ F_2^V \end{bmatrix} = 0$$

The maps $\Phi_3 : \mathbb{R}^{2n+6} \supset D_1 \rightarrow \mathbb{R}^{4n+12}$ and $\Phi_4 : \mathbb{R}^{2n+6} \supset D_1 \rightarrow \mathbb{R}^{5 \times 2}$ are defined as follows:

$$\Phi_3 : u_1 \rightarrow y_1 = \Phi_3(u_1) \hat{=} \begin{bmatrix} T_1^V \\ T_2^V \\ T_1^W \\ T_2^W \\ P_1^V \\ P_2^V \\ \{x_{1,k}^V\}_{k=1}^n \\ \{x_{2,k}^V\}_{k=1}^n \\ P_1^V \\ P_2^V \\ \{x_{1,k}^V\}_{k=1}^n \\ \{x_{2,k}^V\}_{k=1}^n \\ h_{PR}(T_1^W, P_1^V, \{x_{1,k}^V\}_{k=1}^n) \\ h_{PR}(T_2^W, P_2^V, \{x_{2,k}^V\}_{k=1}^n) \\ h_{PR}(T_1^V, P_1^V, \{x_{1,k}^V\}_{k=1}^n) \\ h_{PR}(T_2^V, P_2^V, \{x_{2,k}^V\}_{k=1}^n) \end{bmatrix} \in \mathbb{R}^{4n+12}$$

$$\Phi_4 : u_1 \rightarrow \Phi_4(u_1) \hat{=} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ h_1^W - h_1^V & 0 \end{bmatrix} \in \mathbb{R}^{5 \times 2}, \text{ and } y_2 = \begin{bmatrix} F_1^W \\ F_2^W \\ F_1^V \\ F_2^V \\ \dot{Q} \end{bmatrix} = \Phi_4(u_1)u_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ h_1^W - h_1^V & 0 \end{bmatrix} \begin{bmatrix} F_1^W \\ F_2^W \end{bmatrix}$$

The IDEAS information maps for stream-point load heat exchangers, where the stream is always designated as first, are then defined as follows. Let $T_1^V, T_1^W, T_2, P_1^V, P_1^W$ be the unit's outlet stream temperature (K), unit's inlet stream temperature (K), point load's temperature (K), unit's outlet stream pressure (bar), and unit's inlet stream pressure (bar) respectively, and let $\{x_{1,k}^V\}_{k=1}^n$,

$\{x_{1,k}^W\}_{k=1}^n$ be the kth species' mass fraction of the unit's outlet stream and kth species' mass fraction of the unit's inlet stream respectively. Let also h_1^V, h_1^W be the outlet stream's specific enthalpy (kJ/kg), and inlet stream's heat flow (kJ/kg) respectively (the subscript PR represents the Peng-Robinson equation of state model). Finally, let F_1^W, F_1^V be the ith unit inlet stream's flow rate (kg/s), and ith unit outlet stream's flow rate (kg/s) respectively, and $\dot{Q}$ be the unit's heat load (kJ/s):

$$u = \begin{bmatrix} u_1^T & | & u_2^T \end{bmatrix}^T = \begin{bmatrix} T_1^V & T_1^W & T_2 & P_1^V & \{x_{1,k}^V\}_{k=1}^n & | & F_1^W \end{bmatrix}^T$$

$$y = \begin{bmatrix} y_1^T & | & y_2^T \end{bmatrix}^T = \begin{bmatrix} T_1^V & T_1^W & T_2 & P_1^V & \{x_{1,k}^V\}_{k=1}^n & P_1^W & \{x_{1,k}^W\}_{k=1}^n & h_1^W & h_1^V & | & F_1^W & F_1^V & \dot{Q} \end{bmatrix}^T$$

$$\text{where } u_1 \in D_1 = \left\{ \begin{array}{l} u_1 = \begin{bmatrix} T_1^V & T_1^W & T_2 & P_1^V & \{x_{1,k}^V\}_{k=1}^n \end{bmatrix}^T \in \mathbb{R}^{n+4} : \\ T_1^V \geq 0, T_1^W \geq 0, T_2 \geq 0, P_1^V \geq 0, \sum_{k=1}^n x_k^V = 1, x_k^V \geq 0 \ \forall k = 1, n \end{array} \right\}$$

$$u_2 \in D_2 \triangleq \left\{ u_2 = \begin{bmatrix} F_1^W \end{bmatrix}^T \in \mathbb{R} : F_1^W \geq 0 \right\}$$

No map Ψ_1 need be defined for the considered stream-point load heat exchanger model.

The maps $\Phi_3 : \mathbb{R}^{n+4} \supset D_1 \rightarrow \mathbb{R}^{2n+7}$ and $\Phi_4 : \mathbb{R}^{n+4} \supset D_1 \rightarrow \mathbb{R}^{3 \times 1}$ are defined as follows:

$$\Phi_3 : u_1 \rightarrow y_1 = \Phi_3(u_1) \triangleq \begin{bmatrix} T_1^V \\ T_1^W \\ T_2 \\ P_1^V \\ \{x_{1,k}^V\}_{k=1}^n \\ P_1^V \\ \{x_{1,k}^V\}_{k=1}^n \\ h_{PR}\left(T_1^W, P_1^V, \{x_{1,k}^V\}_{k=1}^n\right) \\ h_{PR}\left(T_1^V, P_1^V, \{x_{1,k}^V\}_{k=1}^n\right) \end{bmatrix} \in \mathbb{R}^{2n+7}$$

$$\Phi_4 : u_1 \rightarrow \Phi_4(u_1) \triangleq \begin{bmatrix} 1 \\ 1 \\ h_1^W - h_1^V \end{bmatrix} \in \mathbb{R}^{3 \times 1}, \text{ and } y_2 = \begin{bmatrix} F_1^W \\ F_1^V \\ \dot{Q} \end{bmatrix} = \Phi_4(u_1)u_2 = \begin{bmatrix} 1 \\ 1 \\ h_1^W - h_1^V \end{bmatrix} \begin{bmatrix} F_1^W \end{bmatrix}$$

The IDEAS information maps, for point load-point load heat exchangers with the cold point load designated with a superscript C and the hot point load with a superscript H, are then defined as follows. Let T^C, T^H be the cold point-load temperature (K), and hot point-load temperature (K) respectively, and $\dot{Q}$ be the unit's heat load (kJ/s).

$$u = \begin{bmatrix} u_1^T & | & u_2^T \end{bmatrix}^T = \begin{bmatrix} T^C & T^H & | & \dot{Q} \end{bmatrix}^T$$

$$y = \begin{bmatrix} y_1^T & | & y_2^T \end{bmatrix}^T = \begin{bmatrix} T^C & T^H & | & \dot{Q} \end{bmatrix}^T$$

where $u_1 \in D_1 \triangleq \left\{ u_1 = \begin{bmatrix} T^C & T^H \end{bmatrix}^T \in \mathbb{R}^2 : T^C \geq 0, T^H \geq 0 \right\}$, $u_2 \in D_2 \triangleq \left\{ u_2 = \begin{bmatrix} \dot{Q} \end{bmatrix}^T \in \mathbb{R} : \dot{Q} \geq 0 \right\}$.

No maps Ψ_1 , Φ_3 , or Φ_4 need be defined for the considered point load-point load heat exchanger model.

Having established the applicability of IDEAS to all considered unit operation models, the structure of the process network is discussed next. The process network is decomposed into

Figure 3: IDEAS representation of a process flowsheet

several subnetworks as shown below in Figure 3. First, a distribution network (DN) where stream splitting and mixing occurs. Then, a heat exchange network (HEN) is considered as outlined in the heat exchanger section above. All unit operations (aside from heat exchangers) are included in an operator network (OP). Finally, a mixing network (MIX) is employed to account for the mixing of process unit outlet streams with identical states, as there is no benefit in allowing streams with the same state to enter the DN at different locations.

A linear objective is considered in the proposed IDEAS formulation, which can be

generally presented as $\sum_{i=1}^{N_{HU}} C_i \dot{Q}_{HU_i}$. This objective function can be used to quantify the varying

costs of the hot utilities loads ($\dot{Q}_{HU_i}$) necessary for the synthesized network through a change in the cost coefficients C .

IDEAS Mathematical Formulation

The above presented mathematical models of all considered processes (reactors, separators, etc.) are combined to yield the following IDEAS mathematical formulation. Let $F_i^U, F_s^V, F_l^W, F_i^X$, be the mass flow rates (kg/s) of the i th DN inlet, s th process unit outlet, l th process unit inlet, and i th MIX outlet respectively; let $F_p^Y, F_p^{Y,l}, F_p^{Y,u}$ be the mass flow rates (kg/s) of the p th DN outlet, p th lower limit DN outlet, and p th upper limit DN outlet respectively; let $F_{l,i}^{WU}, F_{l,i}^{WX}, F_{p,i}^{YU}, F_{p,i}^{YX}$ be the mass flow rates (kg/s) of the i th DN inlet to l th process unit inlet, i th MIX outlet to l th process unit inlet, i th DN inlet to p th DN outlet, and i th MIX outlet to p th DN outlet respectively, and $f_{l,k}^W$ be the mass flow rate of the l th OP inlet's k th species (kg/s). Let also, H^W be the total enthalpy flow of the process unit inlet (kJ/s), and $h_i^U, h_i^V, h_i^W, h_i^X$ be the specific enthalpy (kJ/kg) of the i th DN inlet, i th process unit outlet, i th process unit inlet, and i th MIX outlet respectively; let $h_p^Y, h_p^{Y,l}, h_p^{Y,u}$ be the specific enthalpy (kJ/kg) of the p th DN outlet, p th DN outlet lower limit, and p th DN outlet upper limit (kJ/kg) respectively. Let also, $N_{DN_i}, N_{DN_o}, N_{OP_i}, N_{OP_o}$ be the number of inlet streams in the DN, outlet streams in the DN, inlet streams in the OP, and outlet streams in the OP respectively; let $N_{HEN_i}, N_{HEN_o}, N_{MIX_i}, N_{MIX_o}$ be the number of inlet streams in the HEN, outlet streams in the HEN, inlet streams in the MIX, and outlet streams in the MIX respectively. Let also S^W (kJ/s K) be the total entropy flow for the process unit inlet (kJ/s K), and s_i^U, s_i^X be the specific entropy (kJ/kg K) for the process unit inlet, and process unit outlet respectively. Let also $x_{i,k}^U, x_{i,k}^V, x_{i,k}^W, x_{i,k}^X$ be the k th species mass fraction of

the i th DN inlet, i th process unit outlet, i th process unit inlet, and i th MIX outlet respectively; let

$x_{p,k}^Y, x_{p,k}^{Y,l}, x_{p,k}^{Y,u}$ be the k th species mass fraction of the p th DN outlet, p th DN outlet lower limit,

and p th DN outlet upper limit respectively, and $P_i^U, P_s^V, P_l^W, P_i^X, P_p^Y$ be the pressure (bar) of the

i th DN inlet, s th process unit outlet, l th process unit inlet, i th MIX outlet, and p th DN outlet

respectively. Finally, let $\lambda_{p,i}^{YU}, \lambda_{l,i}^{WU}, \lambda_{p,i}^{YX}, \lambda_{l,i}^{WX}$ be the flags that denote the existence of flow from the

i th DN inlet to the p th DN outlet, from the i th DN inlet to the l th OP inlet, from the i th MIX

outlet to the p th DN outlet, and from the i th MIX outlet to the l th OP inlet respectively; let

$\lambda_{l,i}^{HU}, \lambda_{l,i}^{HX}, \lambda_{l,s}^{XV}$ be the flags that denote the flow from the i th DN inlet to the l th HEX inlet, from

the i th MIX outlet to the l th HEX outlet, and from the s th process unit outlet to the i th MIX inlet

respectively.

$$\nu \triangleq \inf \sum_{i=1}^{N_{HU}} C_i Q_{HU_i}$$

Subject to

$$F_i^U = \sum_{p=1}^{N_{DN_O}} \lambda_{p,i}^{YU} F_{p,i}^{YU} + \sum_{l=1}^{N_{OR_i}} \lambda_{l,i}^{WU} F_{l,i}^{WU} + \sum_{l=1}^{N_{HEN_i}} \lambda_{l,i}^{HU} F_{l,i}^{HU} \quad \forall i=1, N_{DN_i} \quad (1)$$

$$F_i^X = \sum_{s=1}^{N_{MIX_i}} \lambda_{s,i}^{XV} F_s^V = \sum_{p=1}^{N_{DN_O}} \lambda_{p,i}^{YX} F_{p,i}^{YX} + \sum_{l=1}^{N_{OR_i}} \lambda_{l,i}^{WX} F_{l,i}^{WX} + \sum_{l=1}^{N_{HEN_i}} \lambda_{l,i}^{HX} F_{l,i}^{HX} \quad \forall i=1, N_{MIX_O} \quad (2)$$

$$F_p^{Y,l} \leq \sum_{i=1}^{N_{DN_i}} \lambda_{p,i}^{YU} F_{p,i}^{YX} + \sum_{i=1}^{N_{MIX_O}} \lambda_{p,i}^{YX} F_{p,i}^{YX} \leq F_p^{Y,u} \quad \forall p=1, N_{DN_O} \quad (3)$$

$$\left[\begin{array}{c} \sum_{i=1}^{N_{DN_i}} \lambda_{p,i}^{YU} F_{p,i}^{YU} + \\ \sum_{i=1}^{N_{MIX_O}} \lambda_{p,i}^{YX} F_{p,i}^{YX} \end{array} \right] x_{p,k}^{Y,l} \leq \left\{ \begin{array}{c} \sum_{i=1}^{N_{DN_i}} \lambda_{p,i}^{YU} F_{p,i}^{YU} x_{i,k}^U + \\ \sum_{i=1}^{N_{MIX_O}} \lambda_{p,i}^{YX} F_{p,i}^{YX} x_{i,k}^X \end{array} \right\} \leq \left[\begin{array}{c} \sum_{i=1}^{N_{DN_i}} \lambda_{p,i}^{YU} F_{p,i}^{YU} + \\ \sum_{i=1}^{N_{MIX_O}} \lambda_{p,i}^{YX} F_{p,i}^{YX} \end{array} \right] x_{p,k}^{Y,u} \quad \forall k=1, n \quad \forall p=1, N_{DN_O} \quad (4)$$

$$\left[\begin{array}{c} \sum_{i=1}^{N_{DN_i}} \lambda_{p,i}^{YU} F_{p,i}^{YU} + \\ \sum_{i=1}^{N_{MIX_O}} \lambda_{p,i}^{YX} F_{p,i}^{YX} \end{array} \right] h_p^{Y,l} \leq \left\{ \begin{array}{c} \sum_{i=1}^{N_{DN_i}} \lambda_{p,i}^{YU} F_{p,i}^{YU} h_i^U + \\ \sum_{i=1}^{N_{MIX_O}} \lambda_{p,i}^{YX} F_{p,i}^{YX} h_i^X \end{array} \right\} \leq \left[\begin{array}{c} \sum_{i=1}^{N_{DN_i}} \lambda_{p,i}^{YU} F_{p,i}^{YU} + \\ \sum_{i=1}^{N_{MIX_O}} \lambda_{p,i}^{YX} F_{p,i}^{YX} \end{array} \right] h_p^{Y,u} \quad \forall p=1, N_{DN_O} \quad (5)$$

$$f_{l,k}^W = \sum_{i=1}^{N_{DN_i}} \lambda_{l,i}^{WU} F_{l,i}^{WU} x_{i,k}^U + \sum_{i=1}^{N_{MIX_O}} \lambda_{l,i}^{WX} F_{l,i}^{WX} x_{i,k}^X \quad \forall k=1, n \quad \forall l=1, N_{OR_i} \quad (6)$$

$$H_l^W = \sum_{i=1}^{N_{DN_i}} \lambda_{l,i}^{WU} F_{l,i}^{WU} h_i^U + \sum_{i=1}^{N_{MIX_O}} \lambda_{l,i}^{WX} F_{l,i}^{WX} h_i^X \quad \forall l=1, N_{OR_i} \quad (7)$$

$$S_l^W = \sum_{i=1}^{N_{DN_i}} \lambda_{l,i}^{WU} F_{l,i}^{WU} s_i^U + \sum_{i=1}^{N_{MIX_O}} \lambda_{l,i}^{WX} F_{l,i}^{WX} s_i^X \quad \forall l=1, N_{OR_i} \quad (8)$$

$$F^U \geq 0, F^{YU} \geq 0, F^{WU} \geq 0, F^{HU} \geq 0, F^X \geq 0, F^{YX} \geq 0, F^{WX} \geq 0, F^{HX} \geq 0 \quad (9)$$

Where:

$$\lambda_{p,i}^{YU} = \begin{cases} 1 & \text{if } P_p^Y = P_i^U \\ 0 & \text{otherwise} \end{cases}, \lambda_{l,i}^{WU} = \begin{cases} 1 & \text{if } P_l^W = P_i^U \\ 0 & \text{otherwise} \end{cases}, \lambda_{p,i}^{YX} = \begin{cases} 1 & \text{if } P_p^Y = P_i^X \\ 0 & \text{otherwise} \end{cases}, \lambda_{l,i}^{WX} = \begin{cases} 1 & \text{if } P_l^W = P_i^X \\ 0 & \text{otherwise} \end{cases}$$

$$\lambda_{l,i}^{HU} = \begin{cases} 1 & \text{if } P_l^W = P_i^X, \{x_{l,k}^W\} = \{x_{i,k}^X\}, h_l^W = h_i^X \\ 0 & \text{otherwise} \end{cases}, \lambda_{l,i}^{HX} = \begin{cases} 1 & \text{if } P_l^W = P_i^X, \{x_{l,k}^W\} = \{x_{i,k}^X\}, h_l^W = h_i^X \\ 0 & \text{otherwise} \end{cases}$$

$$\lambda_{i,s}^{XV} = \begin{cases} 1 & \text{if } P_s^V = P_i^X, \{x_{s,k}^V\} = \{x_{i,k}^X\}, h_s^V = h_i^X \\ 0 & \text{otherwise} \end{cases}$$

Next, the proposed IDEAS framework is illustrated on a process intensification case study for natural gas reforming based hydrogen production.

CASE STUDY: PROCESS INTENSIFICATION OF NATURAL GAS REFORMING BASED HYDROGEN PRODUCTION

Steam reforming of natural gas (and other light hydrocarbons) is currently the most economical process for hydrogen production⁵⁶. The commonly accepted reactions for steam reforming of methane are as follows:

Hydrogen is used in refineries as raw material for the hydrocracking of oil aiming at gasoline production. In addition, hydrogen is envisioned to be an energy carrier for vehicular transportation through its use in hydrogen fuel-cell-powered cars. The steam reforming process is typically carried out industrially at around 1100K and is highly endothermic. This large endothermic heat load is provided through the burning of natural gas and other available fuel resources in large furnaces operating at temperatures well above 1200K. Steam reforming has been the subject of process integration studies⁵⁷. As process integration evolves into process intensification⁵⁸, steam reforming is increasingly the focus of process intensification efforts (see⁵⁹ and references therein) aiming to improve the economics of this capital and operating cost intensive process. In this case study, the IDEAS framework is applied to the process intensification of a natural gas reforming based flowsheet for hydrogen production, with an

emphasis on minimizing hot utility cost. Three hot utility temperature levels are considered, with each utility having a different cost coefficient. A particular focus point of the study is to explore whether steam methane reforming based hydrogen production can be feasible, in the presence of a debilitating carbon tax for the use of methane as a fuel (and not as raw material). Separation and capital costs are only indirectly accounted for, to the extent they are reflected in the consumption of the three hot utilities, and will be the focus of a future study. Upper bounds on the use of each hot utility are imposed in some instances, to facilitate the creation of flowsheets with different energy consumption characteristics.

A baseline flowsheet is first created on the UniSim (Honeywell Inc. trademark) software, that captures a traditional design of this process. The Peng Robinson equation of state is used to capture the thermodynamic properties of the gas mixture. Natural gas (1 kmol/hr) and water (2 kmol/hr) enter the flowsheet at 298K. Subsequently, both are compressed to 5 bar through the use of a compressor and a pump. Prior to entering a reformer with outlet temperature 1100K, the water and carbon dioxide undergo heating. The reformer outlet is subsequently fed into a sequence of high temperature shift (650K outlet temperature), low temperature shift (475K outlet temperature) reactors with cooling in between. The resultant stream is then cooled before undergoing water, carbon dioxide and hydrogen separation all at 313K. The water, unreacted methane, and carbon monoxide are recycled to the reformer, while hydrogen (4 kmol/hr) and carbon dioxide (1 kmol/hr) are the flowsheet products.

Figure 4 Flowsheet depiction of a traditional natural gas based hydrogen production process.

External hot utility loads of 216.8 kJ/mol of CH₄ fed, 21.78 kJ/mol of CH₄ fed, and 11.84 kJ/mol CH₄ fed are needed at 1200K, 770K and 420K respectively.

The IDEAS methodology is employed to synthesize alternative flowsheet designs to this traditional flowsheet. Given the aforementioned efficiency in searching the design space, afforded by the employed Gibbs free energy minimization based reactor modeling, low dimensional IDEAS LP approximations are employed which identify intensifying designs in the order of a few minutes. The atomic mass fraction ratios of the reformers assume values in the range of 0.33-0.38 for C/O ratio, and 0.07-0.25 for H/O ratio, which includes the atomic ratios of the aforementioned baseline design. The overall stoichiometry of the traditional flowsheet (1 kmol/hr of CH₄ in, 2 kmol/hr H₂O in, 4 H₂ kmol/hr out, 1 CO₂ kmol/hr out) is imposed on all of these IDEAS designs. Multiple optimization instances are carried out for varying cost coefficient ratios of the three hot utilities. In particular, cost coefficient ratios of $24:2:1 (Q_{HU_1} : Q_{HU_2} : Q_{HU_3})$, 4:2:1, 3:2:1, 2.5:2:1, and 1.2:1:1 are considered, with the cost coefficient of the 420K utility

being 0.00425 \$/kJ. In addition, upper bounds are imposed on the use of each hot utility in some instances.

IDEAS generates several different flowsheets depending on the cost coefficient ratios of the hot utilities. When the cost coefficient ratio is 4:2:1 and 24:2:1, the resulting IDEAS flowsheet contains a reformer that has a load of -5kJ/mol of CH₄ fed. In addition, external hot utility loads of 248 kJ/mol of CH₄ and 32.01 kJ/mol of CH₄ are needed at 770K and 420K respectively. The flowsheet produces pure CO₂ as process by-product as well as 4 moles of pure H₂ per mol of CH₄ fed. Removing the need for a 1200K external hot utility, allows the flowsheet's energy needs to be potentially met through use of renewable energy sources, such as solar concentrated power. As the cost coefficient ratio between the 1200K and 770K utility varies from 2.5:2 to 24:2, the amount of 1200K utility used by the IDEAS flowsheet will decrease from 26.26 kJ/s (for 2.5:2 ratio) to 0 kJ/s (for 4:2 ratios and above). These results are summarized in Table 1 below.

Lowering the hot utility ratio from 4:2:1 to 1.2:1:1 produces several flowsheets. Among them are the flowsheets illustrated in Figure 5 and 6, which are simplifications of IDEAS generated designs (following elimination of small flows that have minor contributions to the flowsheet characteristics). Figure 5 was obtained utilizing the cost coefficient of 2.5:2:1, and Figure 6 was obtained by utilizing a cost coefficient ratio of 1.2:1:1, and utility upper bounds of 50kJ/s (1200 K), and 15kJ/s (770 K). The Figure 5 flowsheet employed a reverse-gas-shift (RGS) reactor, a high-temperature swing reactor (HTS), a low-temperature swing reactor (LTS) and three reformers operating at 1145K, 1145K, and 1100K. The Figure 6 flowsheet employs a reverse-gas-shift (RGS) reactor, and a steam-methane reformer operating at 1050K. Both flowsheets have 1 mol of CH₄ and 2 mols of H₂O as inputs and 1 mol of CO₂ and 4 mols of H₂ as

outlets. Table 2 includes the exit temperature information for all process units in the IDEAS flowsheets depicted below, while Table 3 details the inlets to the 1145K reactor and 1100K reactors utilized in the baseline and IDEAS flowsheets, and Table 4 includes the details of all the process streams depicted in Figure 6. The IDEAS flowsheet depicted in Figure 6 has two reactors present, a reformer operating at 1145K and a reverse-gas-shift reactor operating at 750K. As can be seen from Table 1, it consumes 48.72 kJ/s, 14.56 kJ/s, and 3.00 kJ/s of 1200K, 770K, and 420K hot utilities respectively.

Table 1. Summary Table of Natural Gas Based Hydrogen Production Case Study

Metric	Baseline	IDEAS 24:2:1	IDEAS 4:2:1	IDEAS 3:2:1	IDEAS 2.5:2:1	IDEAS 1.2:1:1
Total Hot Utility Cost (24:2:1) (\$/s)	6.22	0.62				
Total Hot Utility Cost (4:2:1) (\$/s)	1.10		0.62			
Total Hot Utility Cost (3:2:1) (\$/s)	0.83			0.64		
Total Hot Utility Cost (2.5:2:1) (\$/s)	0.71				0.69	
Total Hot Utility Cost (1.2:1:1) (\$/s)	0.35					0.32
HU at 1200K, (kJ/s)	60.3	0	0	3.37	26.26	48.72
HU at 770K, (kJ/s)	6.06	68.97	68.97	66.6	46.73	14.56
HU at 420K, (kJ/s)	3.29	8.9	8.9	7.64	5.14	3.00

Figure 5 Simplified IDEAS flowsheet for natural gas based hydrogen production (2.5:2:1 Cost Coefficient Ratio)

Figure 6 Simplified IDEAS flowsheet for natural gas based hydrogen production (1.2:1:1 Cost Coefficient Ratio, utility bounds)

The use of equilibrium reactors, modeled through the presented Gibbs free energy minimization approach, leaves each reactor's feed completely undefined in terms of species molar composition, imposing only a two dimensional restriction on the feed's atom molar ratios

(H/C, O/C). In turn this allows the employed low dimensional IDEAS representation to explore large portions of the species' state space, and to identify CO-rich reformer feeds that make the reformer exothermic (with over 95% methane conversion) and are constructed from the streams being made available from the reactor/separator universe (H₂O separators, H₂ separators, CO₂ separators, high/low temperature shift reactors, and reverse gas shift reactors) considered in the employed finite dimensional IDEAS representation. Figures 6, and 7 illustrate the dependence of the total utility cost, and the utility consumption respectively on the 1200K utility to 770K utility cost coefficient ratio, for the traditional and the IDEAS designs. At small coefficient ratios, IDEAS generates flowsheets that use a combination of 1200K and 770K utilities to reduce the total external hot utility cost.

Table 2 Process unit outlet temperatures

Temperature (K)							
Reformer (Figure 6)	Reformer 1 (Figure 5)	Reformer 2 (Figure 5)	Reformer 3 (Figure 5)	All Separators	HTS (Figure 5)	LTS (Figure 5)	RGS
1040	1145	1145	1100	313	650	475	750

At coefficient ratios of 4:2 and above, no 1200K utilities are employed in the IDEAS flowsheets. The impact on the utility cost is significant. At coefficient ratio 4:2, the IDEAS utility cost is \$0.62/s, while the baseline design is \$1.10/s. At coefficient ratio 24:2 the total utility cost discrepancy between the two designs is so pronounced (\$6.22/s to \$0.62/s) that it justifies the characterization of IDEAS as a systematic process intensification tool. Table 3 below specifies the molar inlets and outlets of the reactors present in the baseline case, and the IDEAS design for a hot utility coefficient ratio of 24:2.

Table 3 Specifications on the inlet and exit of the reactors utilized in the baseline and IDEAS cases presented.

Mol Inlet	Reformer Inlet (1140K) (IDEAS 24:2 utility ratio)	RGS Inlet (750K) (IDEAS 24:2 utility ratio)	HTS Inlet (650K) (Baseline)	LTS Inlet (475K) (Baseline)	Reformer Inlet (1100K) (Baseline)
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CH4 (kmols/hr)	1.03	0	0.09	0.09	1.09
CO (kmols/hr)	14.64	0.14	0.82	0.33	0.07
CO2 (kmols/hr)	0.22	19.7	0.25	0.74	0
H2O (kmols/hr)	17.7	0	1	0.51	2.25
H2 (kmols/hr)	0.27	22.9	3.25	3.74	0
Mol Inlet	Reformer Out (1145 K) (IDEAS)	RGS Out (750K) (IDEAS)	HTS Out (650K) (Baseline)	LTS Out (475K) (Baseline)	Reformer Out (1100K) (Baseline)
CH4 (kmols/hr)	0.03	0	0.09	0.09	0.09
CO (kmols/hr)	8.69	6.08	0.33	0.08	0.82
CO2 (kmols/hr)	7.17	13.72	0.74	1	0.25
H2O (kmols/hr)	9.75	5.94	0.51	0.25	1
H2 (kmols/hr)	10.22	17	3.74	4	3.25

DISCUSSION-CONCLUSIONS

The IDEAS conceptual framework has been put forward as a systematic tool to carry out process intensification studies for total process flowsheets. Efficient use of hot utility resources has been the driving force in this study. The introduction of a Gibbs free energy minimization model allows for the reactor inlets specification in terms of atoms, which has never been presented in process network synthesis. This has allowed the use of process models (e.g. equilibrium reactor models) that enable the systematic search of the large space of alternative process designs. The power of the IDEAS methodology as a process intensification tool is demonstrated on a case study of natural gas reforming based hydrogen production. Minimization of the total external hot utility consumption is pursued for various cost coefficient ratios of the

hot utilities considered. For large cost coefficient ratios of the hottest (1200K) available utility to the second hottest (770K) available utility, IDEAS is able to identify optimal flowsheets that do not require a heat source at 1200K, but rather only at 770K. This comes at the expense of increased separation costs, which however are not a focus of this study, since the flowsheet synthesis method is carried out without commitment to any particular separation technology. Nevertheless, it should be noted that pressure swing adsorption can be employed to separate high CO content hydrogen mixtures⁶⁰, thus avoiding cryogenic separation methods. The reduction (and often the elimination) of the 1200K utility heat load, while keeping true to the energy conservation laws of thermodynamics, necessitates that utility loads at lower temperatures be increased. Since no other material resources are allowed to enter the flowsheet, to ensure a fair comparison to the baseline case, this energy redirection is accomplished by increasing the flowrates through the flowsheet separators. Reducing (or even removing) the 1200K utility load, reduces (or removes) the need for burning natural gas or other fossil fuels to power the reformer, and introduces the possibility of using renewable energy sources, while the natural gas is only used as raw material, and not as an energy source. The HHV of natural gas is 52.2MJ/kg, and with a density of 22kg/Mcf, the HHV of natural gas is 1148.4MJ/Mcf⁶¹. According to the U.S. Energy Information Administration⁶², the average price of natural gas for 2015 was \$12.23/Mcf. Thus, the cost coefficient of natural gas used as an energy source (hot utility) is $\$1.064 \times 10^{-5}/\text{kJ}$ (\$0.038/kWh). A potential renewable (and free on an energy input basis) energy resource that can be brought to bear as a hot utility for the above described natural gas reforming process is concentrated solar power (CSP)⁶³. Solar concentration takes place typically in solar trough and solar tower configurations. A variety of working fluids can be used, including molten salts and synthetic oils. According to the National Renewable Energy Laboratory⁶⁴, solar towers can

currently deliver temperatures of 835K, and are expected to reach 920K by 2020. This is also confirmed by Poullikkas⁶³, who states that CSP tower plants using molten salts can deliver temperatures around 820K. Similarly, solar troughs can currently deliver 720K, and are expected to reach 773K by 2020⁶⁴.

Our future research will focus on the optimization of hydrogen producing flowsheets using alternative objective functions. Among them are total hot/cold/electric utility cost (to account for separator operating costs), and such capital cost measures as heat exchange network total heat transfer area, and reactor capital costs expressed in terms of reactor volume and catalyst weight. More realistic separator technologies will also be considered along with reaction kinetics. In addition, simultaneous reaction and separation will be explored in the future with the inclusion of process units such as membrane reactors within the IDEAS framework.

Figure 7 Cost Coefficient Ratio versus the varying external hot and cold utilities

Figure 8 Total Hot Utility Cost versus the ratio of 1200K:770K utility

Table 4 Specifications on the process flows of the simplified IDEAS generated flowsheet with 1.2:1:1 cost coefficient (Figure 5).

Mole Fraction	VMSR	LMSR	FeedV100	VV100	LV100	LX100	VX100	VX101	LX101	PreHeatMSR	MSRR	MSRRR	CH4 in	H2O in	H2	H2R
CH4	0.0133	0.0133	0.0101	0.0129	0.0000	0.0195	0	0	0.0560	0.0253	0.0253	0.0253	1	0	0	0
CO	0.1686	0.1686	0.1540	0.1970	0.0000	0.2938	0.0059	0	0.8448	0.3821	0.3821	0.3828	0	0	0	0
CO2	0.1312	0.1312	0.2638	0.3374	0.0006	0.0051	0.9941	0	0.0146	0.0069	0.0069	0.0069	0	0	0	0
H2O	0.2703	0.2703	0.2303	0.0152	0.9994	0.0228	0	0	0.0657	0.5771	0.5771	0.5764	0	1	0	0
H2	0.4166	0.4166	0.3419	0.4375	0.0000	0.6588	0	1	0.0189	0.0086	0.0086	0.0086	0	0	1	1
	CO2	CO2R	RGSPH	RGSFeed	RGSV	RGSL	RR	3P	3PT	4P	4PT	VSC	3PP	4PP	RMSR	flas
CH4	0	0	0	0	0.0000	0.0000	0.0000	1	1	0	0	0.0133	1	0	0.0253	0.0101
CO	0.0059	0.0059	0.0046	0.0046	0.1080	0.1080	0.1078	0	0	0	0	0.1686	0	0	0.3821	0.1540
CO2	0.9941	0.9941	0.7865	0.7865	0.6832	0.6832	0.6835	0	0	0	0	0.1312	0	0	0.0069	0.2638
H2O	0	0	0	0	0.1033	0.1033	0.1033	0	0	1	1	0.2703	0	1	0.5771	0.2303
H2	0	0	0.2088	0.2088	0.1055	0.1055	0.1054	0	0	0	0	0.4166	0	0	0.0086	0.3419
	VMSR	LMSR	FeedV100	VV100	LV100	LX100	VX100	VX101	LX101	PreHeatMSR	MSRR	MSRRR	CH4 in	H2O in	H2	H2R
Vapour Fraction	1	0	0.781467	1	0	0.991973	1	1	0.948745	0.429405505	1	1	1	0	1	1
Temperature (K)	1050	1050	313	313	313	313	313	313	313	313	1040	1040	298	298	313	313
Pressure (bar)	5	5	5	5	5	5	5	5	5	5	5	5	1	1	5	5
Molar Flow (kgmole/h)	10.55	0	13.88	10.85	3.03	7.20	3.64	4.70	2.50	5.54	5.54	5.55	1	2	4	0.70
Mass Flow (kg/s)	0.0481	0	0.0807	0.0655	0.0152	0.0210	0.0445	0.0026	0.0184	0.0336	0.0336	0.0337	0.0045	0.0100	0.0022	0.0004
Heat Flow (kJ/s)	-324.3	0	-718.8	-478.6	-240.2	-82.83	-396.5	0.5511	-84.25	-324.47	-246.4	-246.7	-20.81	-159.0	0.4693	0.0819
	CO2	CO2R	RGSPH	RGSFeed	RGSV	RGSL	RR	3P	3PT	4P	4PT	VSC	3PP	4PP	RMSR	flas
Vapour Fraction	1	1	1	1	1	0	1	1	1	0	1	1	1	1	1	1
Temperature (K)	313	313	312.3	750	750	750	750	459.2	1040	298	1040	750	700	700	650	750
Pressure (bar)	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
Molar Flow (kgmole/h)	1	2.64	3.34	3.34	3.34	0	3.33	1	1	2	2	10.55	1	2	5.54	13.88
Mass Flow (kg/s)	0.0122	0.0323	0.0326	0.0326	0.0326	0	0.0325	0.0045	0.0045	0.0100	0.0100	0.0481	0.0045	0.0100	0.0336	0.0807
Heat Flow (kJ/s)	-108.8	-287.7	-287.62	-270.73	-267.1	0	-266.3	-19.04	-9.34	-159.01	-119	-356.5	-15.62	-126.5	-268.8	-622.8

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