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An MILP model for the design of shale gas industrial parks

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Abstract

A multi-period model for the development of a sustainable industrial park based on shale gas as raw material is presented. From techno-economic data for processes to produce chemicals such as ethylene, benzene, syngas, methanol, butadiene and propylene, a multi-period mixed-integer linear programming model was developed. Driven by exogenous demands for chemicals and aiming to maximize the expected revenue of the industrial park, the model was applied for a 10-year development period to provide an optimal structure of production processes that make best use of shale gas as a primary feedstock. As a result, a program of selected technologies and capacity expansions for each chemical was obtained, along with the benefits to integrate a sustainable industrial park that uses the internal production of a given chemical to serve as a raw material for a downstream process. Water integration is examined as part of the sustainability benefits of the industrial park. From an economic viewpoint, it is shown that such an industrial complex provides a significant incentive for shale gas monetization.

Keywords: Shale gas; industrial park; optimization; MILP

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Nomenclature

Acronyms

<i>BCFD</i>	Billions of cubic feet per day
<i>d</i>	Days
<i>GJ</i>	Giga Joule
<i>MM\$</i>	Millions of dollars
<i>MMBtu</i>	Millions of British Thermal Unit
<i>MMGJ</i>	Millions of Giga Joule
<i>MMSCFD</i>	Millions of standard cubic feet per day
<i>MMT</i>	Millions of metric tonnes
<i>MMTCO₂e</i>	Millions of metric tonnes of CO ₂ equivalent emissions
<i>SCFD</i>	Standard cubic feet per day
<i>T</i>	Metric tonnes
<i>MWh</i>	Megawatt-hour
<i>y</i>	Years

Indices

<i>c</i>	Fixed cost intervals
<i>i</i>	Chemical components
<i>j</i>	Process
<i>t</i>	Time periods
<i>u</i>	Utilities

Parameters

$\alpha_{i,j}^{in}$	Input coefficient for the consumption of chemical <i>i</i> in process <i>j</i> [T/T of main product]
$\alpha_{i,j}^{out}$	Output coefficient for the production of chemical <i>i</i> in process <i>j</i> [T/T of main product]
A_i	Cost of chemical <i>i</i> [\$/T]
B_u	Cost of utility <i>u</i> [\$/GJ]
$CapI_j^{max}$	Maximum installation capacity by plant of process <i>j</i> [MMT/y]
$CapI_j^{min}$	Minimum installation capacity by plant of process <i>j</i> [MMT/y]
$CapE_{j,t,c}^{Lo}$	Lower bound of expansion capacity plant of process <i>j</i> in time <i>t</i> with capacity localized in section <i>c</i> [MMT/y]
$CapE_{j,t,c}^{Up}$	Upper bound of expansion capacity plant of process <i>j</i> in time <i>t</i> with capacity localized in section <i>c</i> [MMT/y]
$CapI_{j,t,c}^{Lo}$	Lower bound of installation capacity plant of process <i>j</i> in time <i>t</i> with capacity localized in section <i>c</i> [MMT/y]
$CapI_{j,t,c}^{Up}$	Upper bound of installation capacity plant of process <i>j</i> in time <i>t</i> with capacity localized in section <i>c</i> [MMT/y]

$CO_2e_j^{elec}$	CO ₂ equivalent emissions due to electricity consumption in process j [TCO ₂ e/T of product]
$CO_2e_j^{heat}$	CO ₂ equivalent emissions due to heating utility in process j [TCO ₂ e/T of product]
$dem_{i,t}$	Demand of chemical i in time t [MMT/y]
$fix_{j,c}$	Fixed capital investment of process j with capacity localized in section c [MM\$]
$InfR$	Inflation rate
$IntR$	Interest rate
$S^{SG,up}$	Upper bound of shale gas supply [MMT/y]
SG^{cost}	Shale gas price as raw material [\$/T]
SG^{proC}	Shale gas processing cost [\$/T of shale gas fed]
$uti_{j,u}^{con}$	Consumption of utilities u in process j [GJ/T]
$var_{j,c}$	Variable capital investment of process j with capacity localized in section c [MM\$]
x_i^{SG}	Shale gas yield

Variables

AFC_t	Annualized fixed capital investment cost [MM\$/y]
$Cap_{j,t}$	Capacity operation plant of process j in time t [MMT/y]
$CapE_{j,t}$	Capacity expansion plant of process j in time t [MMT/y]
$CapI_{j,t}$	Capacity installation plant of process j in time t [MMT/y]
CO_2e_t	CO ₂ equivalent emissions in time t [MMTCO ₂ e/y]
CO_2ee	Total CO ₂ equivalent emissions [MMTCO ₂ e]
$F_{i,j,t}$	Total raw material input of chemical i to process j in time t [MMT/y]
$F_{i,j,t}^{SG}$	Amount of chemical i from shale gas fed to process j in time t [MMT/y]
$FCI_{j,t}$	Fixed capital investment of build a plant of process j in time t [MM\$]
$FCIE_{j,t}$	Fixed capital investment of build a capacity expansion plant of process j in time t [MM\$]
$I_{i,j,t}^{raw}$	Imported raw material of chemical i to process j in time t [MMT/y]
$income_t$	Incomes in time t [MM\$/y]
m_t^{SG}	Shale gas mass flow in time t [MMT/y]
NPV	Net present value [MM\$]
$O_{i,j,t}$	Production of chemical i from process j in time t [MMT/y]
$O_{i,t}^{SG}$	Amount of chemical i from shale gas does not fed in any process j in time t [MMT/y]
$P_{i,t}$	Production of chemical i in time t [MMT/y]
$profit_t$	Profit in time t [MM\$/y]
$R_{i,j,t}$	Recirculation of chemical i to process j in time t [MMT/y]

raw_t	Raw material cost in time t [MM\$/y]
$S_{i,t}^{SG}$	Amount of chemical i from shale gas supply in time t [MMT/y]
SG_i^{pro}	Shale gas processing cost in time t [MM\$/y]
$TFCI$	Total fixed capital investment cost [MM\$]
$Ton_{j,t}^{prod}$	Tonnes of production in process j in time t [MMT of main product/y]
uti_t	Utilities cost in time t [MM\$/y]
$W_{j,t,c}$	Disaggregated binary variable of build or not build a plant of process j in time t with capacity localized in section c
$WE_{j,t,c}$	Disaggregated binary variable of build or not build a capacity expansion plant of process j in time t with capacity localized in section c
$Y_{j,t}$	Binary variable of build or not build a plant of process j in time t
$YE_{j,t}$	Binary variable of build or not build a capacity expansion plant of process j in time t
$YO_{j,t}$	Binary variable when plant of process j is operating in time t

Introduction

Industrial parks provide a valuable alternative for the design of sustainable transformation systems since they may share common raw materials and facilitate the transfer of products from a given process that can serve as feedstocks for another unit. In this sense, one interesting option to analyze for the development of an industrial park is the use of shale gas as a common raw material, given that its recent discoveries have promoted its use as an important source of energy and value-added chemicals. Shale gas is an unconventional dry natural gas obtained from ultra-low permeability shale formations¹. Shale gas resources differ from conventional natural gas ones in factors such as a deeper location, the need for special techniques such as fracking and horizontal drilling for its commercial production, and a wider chemical composition (Table 1)¹.

Similar to natural gas, shale gas can also be monetized via integrated supply chains into a variety of products including fuels, chemicals, fertilizers, and petrochemicals^{2,3}. Each of the hydrocarbon components can be converted into basic, intermediate and final products. For instance, with one of the largest natural gas reserves in the world, the Qatar industry has developed an important supply chain that includes a highly integrated network of intermediate and final products^{2–4}. With the understanding that chemical composition of shale gas varies from one well to another (Table 2) and that its composition changes during the production

history of the well¹, each shale gas basin offers opportunities and challenges to incorporate the use of shale gas as part of a current infrastructure that depends on conventional natural gas. The creation of viable supply chains for monetizing shale gas may include the development of industrial parks that takes advantage of available resources and supply characteristics of a given region of interest. For an economic perspective, the price differential between shale from the well head with respect to pipeline-quality natural gas needs to be determined, as shown by Ehlinger et al.⁵ for the case of Barnett shale gas.

Different shale gas processing technologies have been analyzed, which can provide the basis for their integration in the form of industrial parks that meet specific demands of major chemicals such as benzene⁶, methanol⁷ ethylene⁸ and olefins⁹. A review for opportunities of shale gas monetization has been reported². Modeling efforts tied to optimization frameworks for shale gas processing have also been reported, including superstructure formulations for the production of liquids of natural gas (LNG), gas to liquids (GTL) and methanol⁴, and for light olefins based on Marcellus shale gas feed¹⁰.

From the literature review, one can observe that several designs have been proposed for the production of individual value-added chemical from shale gas. In this work, we take a set of commercially valuable products and formulate an optimization model that can be used for the planning of sustainable industrial parks that make use of shale gas as a common feedstock.

Problem statement

Given a set of products with established demand levels driven by their high economic value, and a set of technologies available for their manufacture from shale gas as a primary raw material, it is desired to find the structure of an integrated multi-period production network that includes technology selection and capacity expansion plants over time that maximizes the expected economic revenue.

Technology catalog

A search for technical and economic data for processes that transform shale was into higher value-added products was conducted. Specifically, processes to produce benzene, syngas, methanol, dimethyl ether (DME), ethylene, propylene, butadiene, ammonia and urea were chosen. The basic technologies considered here are as follows.

Benzene can be produced from direct methane aromatization (DMA). Syngas and ethylene can also be produced directly from methane. For syngas, five reforming processes are considered: auto thermal reforming (ATR), combined reforming (CR), dry reforming (DR), partial oxidation (POX), and steam methane reforming (SMR). Syngas is a major intermediate for the production of methanol, DME, and olefins. In addition to the route from syngas, DME can also be produced by methanol dehydration (MD). Ethylene is a major building block of petrochemicals, and nine production processes were considered for its manufacture: methane cracking (MC), oxidative coupling of methane (OCM), non-oxidative coupling of methane (NOCM), methanol to olefins (MTO), ethane cracking (EC) with two variants (one that includes an external refrigerant and the other one with the co-production of such refrigerant), an integration of EC and propane dehydrogenation (PD) process, a cracking process using a ethane-propane mixture (EPM) as raw material, and propane cracking (PC). Propylene, another major intermediate petrochemical, can be produced via propane dehydrogenation (PD). Butadiene can be obtained by dimerization of ethylene (DOE), for which two options based on different operation conditions can be considered. For ammonia production, the Haber-Bosch (HB) process was selected. Finally, urea production from ammonia completes the set of transformation processes considered in this work. The list of chemical processes is given in Table 3. Fig. 1 gives an overall view of the network, with the production alternatives for each transformation process, while Fig. 2 shows a compact representation of the superstructure that results from the integration of the supply-transformation-demand production chain.

Design of the superstructure

A superstructure that contains N ($=29$) chemicals involved in M ($=23$) processes was constructed. The variables associated to flow of material for the production network are shown in Fig. 3. For each chemical i at time t , the industry takes an exogenous shale gas supply $S_{i,t}^{SG}$ (output from first block and input to node 1 in Figure 3) with composition x_i^{SG} , and unknown flow m_i^{SG} . The shale gas supply is first separated into its main chemical components, which can be fed to process j as $F_{i,j,t}^{SG}$, or sent out from the network as $O_{i,t}^{SG}$ (mass balance in node 1 in Figure 3). Imported raw materials $I_{i,j,t}^{raw}$ are available to meet the feedstock needs $F_{i,j,t}$, if

needed (output from node 2 in Figure 3). $O_{i,j,t}$ contains the chemical products manufactured in each process j ; the chemicals produced can be recycled to the network as $R_{i,j,t}$ or sent out for commercialization as $P_{i,t}$ (mass balance in node 3 in Figure 3). It is desired to find the optimal structure of an industrial park based on shale gas that meets the products exogenous demand with maximum profit.

Tables 4 and 5 include the mass balance coefficients for the technologies, while data related to energy consumption and investment requirements are given in Tables 6 and 7. For the investment data, base values for reported technologies were used, adjusted to world scale facilities using the 6/10 rule¹¹, and updated to the year 2019 using the Chemical Engineering Plant Cost Index (CEPCI)¹². The problem was formulated as a mixed-integer linear programming (MILP) optimization model and solved using the GAMS software.

Mathematical modeling

The objective of the model consists of selecting which plants, among those included in the superstructure, must be constructed and operated inside the industrial park, when the constructions must start, and associated to forecasted increase in product demands when and which plants should be expanded. To evaluate the performance of the industrial park, a 10-year planning horizon was taken, discretized into one-year periods.

The following sets are used in the model formulation.

- N { i | i is a chemical that can appear in any part of the industrial complex}
- M { j | j is a process in the superstructure}
- U { u | u is a utility used by any of the processes}
- T { t | t is a time period}

Ten different utilities are considered. For cooling duties, water at 30 °C, chilled water at 5 °C, and four types of refrigerants available at -20, -50, -100, and -150 °C are assumed. For heating tasks, low pressure steam at 160 °C and 5 bar, high pressure steam at 254 °C and 41 bar, and fuel are considered. Electricity is taken as power.

The net present value of profit (NPV) is used as a measure of the network profitability,

$$NPV = \sum_{t \in T} profit_t \cdot (1 + IntR)^{-t} \quad (1)$$

Where $IntR$ is the interest rate, taken as 10%. The annual profit is the difference between the income obtained from the sales of products and the annual expenses, which include costs due to shale gas pre-processing (SG_t^{pro}), raw materials (raw_t), utilities (uti_t), and the annualized capital investment (AFC_t):

$$profit_t = income_t - (SG_t^{pro} + raw_t + uti_t + AFC_t) \quad \forall t \in T \quad (2)$$

Earnings are given by total production $P_{i,t}$ sold at a unit price A_i :

$$income_t = \sum_{i \in N} P_{i,t} \cdot A_i \cdot (1 + InfR)^t \quad \forall t \in T \quad (3)$$

Where $InfR$ is the inflation rate, taken as 2.5%.^{11,13}

The mass flow of shale gas fed (m_t^{SG}) to the network has a pre-processing cost per metric ton of shale gas (SG^{proC}):

$$SG_t^{pro} = m_t^{SG} \cdot SG^{proC} \cdot (1 + InfR)^t \quad \forall t \in T \quad (4)$$

The raw material cost includes the amount of shale gas purchased at a price SG^{cost} plus the amount of imported raw material ($I_{i,j,t}^{raw}$) bought at a unit price A_i :

$$raw_t = [m_t^{SG} \cdot SG^{cost} + \sum_{i \in N} \sum_{j \in M} I_{i,j,t}^{raw} \cdot A_i] \cdot (1 + InfR)^t \quad \forall t \in T \quad (5)$$

Utility costs are calculated from the unit consumption in each process j ($uti_{j,u}^{con}$) with a unit cost B_u , multiplied by the process production rate ($Ton_{j,t}^{prod}$):

$$uti_t = \sum_{j \in M} \sum_{u \in U} uti_{j,u}^{con} \cdot B_u \cdot Ton_{j,t}^{prod} \cdot (1 + InfR)^t \quad \forall t \in T \quad (6)$$

The annualized capital investment is calculated with Eq. 7.¹¹

$$AFC_t = FCI \cdot \left[\frac{IntR \cdot (1 + IntR)^{|t|}}{(1 + IntR)^{|t|} - 1} \right] \quad \forall t \in T \quad (7)$$

The total shale gas mass flow is limited by the exogenous gas supply $S^{SG,up}$,

$$m_t^{SG} \leq S^{SG,up} \quad \forall t \in T \quad (8)$$

The flow of each component in the shale gas is calculated with Eq (9).

$$m_t^{SG} \cdot x_i^{SG} = S_{i,t}^{SG} \quad \forall i \in N, \forall t \in T \quad (9)$$

The total mass flow of chemical i in a given time period is equal to the amount in the shale gas minus any amount of by-passed chemical, Eq (10). Note that Eq (10) is a mass balance in the first splitter of the superstructure (node 1 in Figure 3).

$$\sum_{j \in M} F_{i,j,t}^{SG} = S_{i,t}^{SG} - O_{i,t}^{SG} \quad \forall i \in N, \forall t \in T \quad (10)$$

The feedstocks entering a given process in the network may include chemicals included in the shale gas, imported raw materials and any recycled amount,

$$F_{i,j,t} = F_{i,j,t}^{SG} + I_{i,j,t}^{raw} + R_{i,j,t} \quad \forall i \in N, \forall j \in M, \forall t \in T \quad (11)$$

For the decision to build a plant in a period t , a Boolean variable $Y_{j,t}$ is used, which takes the value of 'True' if the plant is built, and 'False' otherwise. The investment cost of each plant is calculated in terms of a reference cost for a base capacity (Table 7). To maintain the linearity of the model, the investment cost is linearized through a piecewise (PW) linear function as follows,

$$\left[\begin{array}{c} Y_{j,t} \\ CapI_j^{\min} \leq CapI_{j,t} \leq CapI_j^{\max} \\ Cap_{j,t} \leq CapI_{j,t} \\ W_{j,t,c} \\ \bigvee_{c \in PW} \left[\begin{array}{c} FCI_{j,t} = fix_{j,c} + var_{j,c} \cdot CapI_{j,t} \\ CapI_{j,t,c}^{Lo} \leq CapI_{j,t} \leq CapI_{j,t,c}^{Up} \end{array} \right] \end{array} \right] \preceq \left[\begin{array}{c} \neg Y_{j,t} \\ CapI_{j,t} = 0 \\ FCI_{j,t} = 0 \end{array} \right] \quad \forall j \in M, \forall t \in T \quad (D1)$$

The Boolean variable ($W_{j,t,c}$) is used to select the linear approximation over the set PW of piecewise linear cost sections (c). Initially a process plant is built with a capacity ($CapI_{j,t}$) between lower and upper bounds.

It is assumed that at most one plant for each chemical can be built,

$$\bigvee_{t \in T} (Y_{j,t}) \leq Z \quad \forall j \in M \quad (12)$$

Where Z is a dummy Boolean variable that takes the value of True if process j is not selected to be built.

After the process is built, an expansion takes place when the increase in demand provides an economic incentive. The following disjunction models the operation and expansion of a chemical plant.

$$\begin{aligned}
 & \left[\begin{array}{c}
 YO_{j,t} \\
 \left. \begin{array}{l}
 F_{i,j,t} = \alpha_{i,j}^{in} \cdot Ton_{j,t}^{prod} \\
 O_{i,j,t} = \alpha_{i,j}^{out} \cdot Ton_{j,t}^{prod} \\
 P_{i,t} = \sum_{j \in M} (O_{i,j,t} - R_{i,j,t})
 \end{array} \right\} \forall i \in N \\
 Cap_{j,t} = Cap_{j,t-1} + CapE_{j,t} \\
 Ton_{j,t}^{prod} \leq Cap_{j,t}
 \end{array} \right] \vee \left[\begin{array}{c}
 \neg YO_{j,t} \\
 F_{i,j,t} = 0 \\
 O_{i,j,t} = 0 \\
 P_{i,t} = 0 \\
 R_{i,j,t} = 0 \\
 Cap_{j,t} = 0 \\
 Ton_{j,t}^{prod} = 0
 \end{array} \right] \forall j \in M, \forall t \in T \\
 & \left[\begin{array}{c}
 YE_{j,t} \\
 CapE_{j,t} \leq 0.5 \cdot CapI_j^{\max} \\
 \left[\begin{array}{c}
 WE_{j,t,c} \\
 FCIE_{j,t} = fixE_{j,c} + varE_{j,c} \cdot CapE_{j,t} \\
 CapE_{j,t,c}^{Lo} \leq CapE_{j,t} \leq CapE_{j,t,c}^{Up}
 \end{array} \right] \vee \left[\begin{array}{c}
 \neg YE_{j,t} \\
 CapE_{j,t} = 0 \\
 FCIE_{j,t} = 0
 \end{array} \right]
 \end{array} \right] \vee \left[\begin{array}{c}
 \neg YE_{j,t} \\
 CapE_{j,t} = 0 \\
 FCIE_{j,t} = 0
 \end{array} \right] \vee \left[\begin{array}{c}
 \neg YO_{j,t} \\
 F_{i,j,t} = 0 \\
 O_{i,j,t} = 0 \\
 P_{i,t} = 0 \\
 R_{i,j,t} = 0 \\
 Cap_{j,t} = 0 \\
 Ton_{j,t}^{prod} = 0
 \end{array} \right] \forall j \in M, \forall t \in T
 \end{aligned} \tag{D2}$$

The disjunction (D2) includes equations related to mass balance (see block 3 of Figure 3 labeled as 'Process j'), and production capacity of a process including expansions; $\alpha_{i,j}^{in}$ and $\alpha_{i,j}^{out}$ are input/output mass balance coefficients. The manufactured chemicals, $P_{i,t}$, can be recycled or sent out of the network for sale. Production is limited by the process capacity.

Implicit in disjunction (D2) are the following conditions.

A plant cannot be expanded if it is not in operation:

$$YE_{j,t} \Rightarrow YO_{j,t} \quad \forall j \in M, \forall t \in T \tag{13}$$

A process plant cannot be operated before it is built, and once it is built it must be operated:

$$YO_{j,t} \Rightarrow \bigvee_{t' \in T | t' \leq t} Y_{j,t'} \quad \forall j \in M, \forall t \in T \tag{14}$$

$$Y_{j,t} \Rightarrow YO_{j,t'} \quad \forall j \in M, \forall (t, t') \in T | t' \geq t \tag{15}$$

A plant cannot be built and expanded in the same time period:

$$Y_{j,t} \vee YO_{j,t} \vee Z_{j,t} \quad (16)$$

Here, Z is a dummy variable that takes the value of 'True' if plant j is neither built nor operated in time period t .

The net production of chemical i is limited by the exogenous demand of the product:

$$P_{i,t} \leq dem_{i,t} \quad \forall i \in N, \forall t \in T \quad (17)$$

As part of the model solution, basic assessment for environmental analysis is conducted through the evaluation of total CO₂ equivalent emissions, CO_2ee , which are calculated using a factor of 0.46 TCO₂e/MWh for electricity ($CO_2e_j^{elec}$) and 0.066 TCO₂e/MMBtu for heating utilities ($CO_2e_j^{heat}$).¹⁴ Process emissions ($\alpha_{CO_2,j}^{out}$) and consumption ($\alpha_{CO_2,j}^{in}$) of CO₂ complete the balance.

$$CO_2ee = \sum_{t \in T} CO_2e_t \quad (18)$$

$$CO_2e_t = \sum_{j \in M} (CO_2e_j^{elec} + CO_2e_j^{heat} + \alpha_{CO_2,j}^{out} - \alpha_{CO_2,j}^{in}) \cdot Ton_{j,t}^{prod} \quad \forall t \in T \quad (19)$$

The model comprises equations 1 to 19 and disjunctions D1 and D2. The solution included the reformulation of disjunctions using the convex hull reformulation technique.^{15–17}

Case study

As the raw material, shale gas produced from the Barnett shale play was assumed. The Barnett shale production has jumped from nearly non existing in 1999 to approximately 4 BCFD in 2008; to keep this growth, the equivalent of 100 MMSCFD have been added to gas processing plants every 3 months for ten years¹⁸. With estimates of 300-350 SCF of gas per ton of shale^{1,18}, and considering a gas processing industry of 100 MMSCFD, an estimate of 0.34 MMT/d of shale gas was taken as an upper limit for the supply of shale raw material.

Chemical and utility prices are reported in Tables 8 and 9. Natural gas prices have ranged from 1.7 to 5.98 \$/MMBtu over the last five years¹⁹. A differential price of 20% between natural gas (C₁) and Barnett shale gas was taken,^{5,20} along with a preprocessing cost of 14.7 \$/T.²⁰ To update prices over time, an inflation rate of 2.5% was assumed.^{11,13}

To set the exogenous demand for chemicals, USA imports over the period 2018-2019 were taken as a basis. Annual average demand growth was estimated from adjusting demand projections. For example, Al-Douri et al.² reported that global methanol demand is expected to grow from 60.7 to 109 MMT from 2013 to 2023, which represents an increase of 79% over a 10-year period; yearly demands were then fixed from that value. Table 10 reports the initial demand and yearly growth assumed for each chemical.

Worldwide scale capacities for each chemical, as reported in Table 7, were taken as maximum values in the model formulation. For a process to be built, it is assumed that its capacity must be at least 20% of the value given in Table 7, and that its production must be at least 60% of the installed capacity. A 10-year time horizon discretized over one-year periods with 330 working days per year was assumed. To annualize the FCI and adjust the NPV to the reference time, an interest rate of 10% was assumed.

Results

The optimal structure of the industrial park provided by the model is shown in Fig. 4. Out of the choices included in the formulation, shale gas monetization into benzene, syngas, methanol, ethylene, propylene, and butadiene was selected. Fig. 5 shows the yearly production of these chemicals. The potential NPV for this development plan is 26,346 MM\$ for the 10-year time horizon. The expected yearly NPV is presented in Fig 6. As far as the environmental analysis, 116.8 MMTCO₂ equivalent emissions was estimated for the production period.

Relevant details on the technology assessment for each production chemical are as follows.

Benzene is produced based on C₁ from shale gas using the direct methane aromatization (DMA) process. Syngas is produced using the steam methane reforming (SMR) technology and used as a raw material for methanol synthesis. The non-oxidative coupling of methane (NOCM) process is selected for the production of ethylene, while butadiene is manufactured via dimerization of ethylene (DOE) at 1273K. Propylene production is made through the propane dehydrogenation (PD) process. Significant amounts of H₂, naphtha, coke, and tail gas are formed as by-products within the production network.

The network is supported by an initial consumption of 26,575 T/d of shale gas, with an increase to 40,267 T/d observed at end of the 10th-year period. Some details of the multi-

period production network are given next, making emphasis on the initial and final production state for each chemical.

- Benzene. The initial capacity is 3,633 T/d, with the plant operating at 95% of its capacity and consuming 6,955 T/d of methane as a raw material. By the end of the 10-year development period, the production of benzene reaches 3,633 T/d, which requires 7,293 T/d of methane. Benzene is also produced as a by-product in the ethylene plant. This combination of processes serves to meet the exogenous demand for benzene of 5,714 T/d for the first year and 7,102 T/d for year 10. Hydrogen, naphtha, and coke are formed as by-products in the benzene plant, in amounts for the first year of 683 T/d, 1,034 T/d, and 974 T/d, respectively; the by-production reaches, respectively, 716 T/d, 1,084 T/d, and 1,021 T/d by year 10.

- Syngas. Syngas is an intermediate for the production of methanol. From the set of reforming techniques, the technology selected for syngas is based on steam methane reforming (SMR). The maximum capacity of syngas at the end of the 10-year period reaches 12,200 T/d. Some details are as follows. The initial capacity is 6,100 T/d, and the process operates at 70% of its capacity, for which 2,175 T/d of methane from shale gas are used as feedstock, and 259 T/d of hydrogen are produced as by-product. To keep up with the internal need for syngas, two expansions of 3,150 T/d each are needed, one in year 2 and the second one in year 4. The use of installed capacity becomes complete after year 5.

- Methanol. The initial capacity for methanol production is 4,400 T/d. Expansions take place in periods 2, 3, 4, and 5, to end the 10-year period with a total production capacity of 13,200 T/d. A consumption of 6,067 T/d of syngas is initially needed, reaching 18,202 T/d by year 10. Starting in year 5, imports of 856 T/d of syngas are needed to supplement the internal production of syngas in the industrial park. To meet the syngas molar relationship in the recycle stream, CO imports are needed in amounts of 83 T/d in year 1, growing to reach 250 T/d in the 10th period. A small amount of tail gas is also produced. The methanol plants work at maximum capacity during the 10-year period.

- Ethylene. The initial production capacity of ethylene is 2,644 T/d, and no expansions are required later. By-products hydrogen, benzene, naphtha, and tail gas are produced in amounts of 4,448 T/d, 3,469 T/d, 4,215 T/d, and 754 T/d, respectively, by year 10. A small amount of ethylene production is recycled to the butadiene plant.

- Propylene. The capacity for propylene production provided by the model for year 1 is 1,013 T/d with no need for expansions. The propylene production needed to meet its exogenous demand is driven by propane from shale gas as feedstock at an initial rate of 784 T/d, reaching 1,183 T/d for the last year. Small amounts of hydrogen, LPG and tail gas are produced.

- Butadiene. Driven by 317 T/d of ethylene, of which 178 are provided by direct recycle from the plant and 139 T/d from the ethylene process, the initial butadiene production amounts to 122 T/d. The final butadiene production of 162 T/d requires 418 T/d of ethylene. The production is based on a butadiene plant with 200 T/d of production capacity. A small amount of tail gas is also produced.

- By-products: The production of by-products reaches 5,937 T/d of hydrogen, 5,300 T/d of naphtha, 3 T/d of LPG, 1,021 T/d of coke, and 961 T/d of tail gas at the end of the development period.

Water and energy nexus

As part of the sustainable operation of the industrial park, the water produced in the network can be potentially recycled to supply some of the overall needs. For this analysis, we assume that the water discharged from any process can be directly recyclable, i.e., adjustments for pollutants content or other factors are not considered. One can identify two processes that consume water, the syngas and the butadiene technologies. In the syngas process, 7,056 T/d of water are needed in year 1 for the reaction with methane to produce syngas in the SMR reactor; from this process, 4,615 T/d of unreacted water are recovered in the output stream. For the last period, the syngas plant requires 19,780 T/d of process water, from which 12,937 T/d are recovered and can be recycled. The butadiene synthesis reaction uses a water quenching tower to reduce hazards in the hot reactor stream, with a water consumption of 408 T/d in the first year, reaching 537 T/d by the 10th year; the amount of water discharged from this process is practically equal to the amount of fresh water required for the reaction.

An overall water balance for the 10-year period, given in Figure 7, indicates that a total amount of 57 MMT of fresh water is needed for syngas and butadiene production, out of which 37.8 MMT of water are potentially recoverable from the discharge of those processes. Therefore, if a direct recycle scheme is implemented, the fresh water consumption can be reduced by 66 percent to 19.2 MMT.

In terms of the energy requirements for the industrial park, the accumulated 10-year breakdown consumption by each plant are given in Table 11 and shown in a comparison chart in Figure 8. One can see that the syngas process has the highest cooling requirements, while the ethylene plant consumes the highest heating utility and is the most power-intensive process from the network.

Sensitivity analysis

Given the noticeable changes in shale gas prices observed in recent times, a sensitivity analysis was carried out to assess the ability of the process to withstand those price changes. From the base value of 3.1 \$/MMBtu, prices of shale gas were assumed to drop as low as 1.36 and raise as high as 4.8 \$/MMBtu (equivalent to \$1.7 to \$6.0 per MMBtu of natural gas prices), and the results are shown in Fig. 9. It can be observed that benzene, ethylene, and butadiene processes show a robust economic profitability, based on their steady plant capacity, despite changes in raw material prices; propylene capacity is practically the same for any price of shale gas. The syngas and methanol plants are the sensitive technologies to changes in shale gas prices; for low prices, the optimal structure shows three syngas expansions, but some of them become gradually nonprofitable as the price of shale gas increases, such that for prices of \$4.8 per MMBtu only one expansion becomes profitable for implementation. For the case of methanol, five expansions are selected for low shale gas prices, while only three show a suitable economic potential at high prices.

The overall economic benefit from the industrial park as a function of the shale gas prices is shown in Fig. 10, in the form of yearly benefits (Fig. 10a) and accumulated profit (Fig. 10b). The results show that a 3.5 times increase in shale gas prices would affect the accumulated net benefit by 37%. Fig. 10 displays the yearly production of chemicals selected by the model in the face of changing shale gas prices.

Conclusions

A model for the development of a shale gas industrial park has been formulated. The model was developed within a multi-period, mixed-integer linear programming framework. A set of 23 different technologies that can produce chemicals such as benzene, syngas, methanol, dimethyl ether, ethylene, propylene, butadiene, ammonia and urea was considered as a basis for the integration of an industrial park based on shale gas as a starting raw material. The

application of the model for a 10-year development period was conducted. From the set of chemicals and their technologies, the selection was based on their economic potential. As a result, the production network begins with the conversion of shale gas to produce benzene, syngas, ethylene and propylene, and methanol and butadiene are then produced from those intermediate chemicals. Based on the economic scenario with base current prices considered in this work, an accumulated net present value for the 10-year period of 26,346 MM\$ was estimated for the optimal production network provided by the model. A sensitivity analysis on the prices of shale gas showed that the industrial park structure offers a fairly robust behavior, since only the production of syngas and methanol was affected as a consequence of changes in shale gas prices. The model was based on the use of the Barnett shale play as the source for shale gas, but its formulation can be adjusted to other regional configuration of shale gas availability.

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Table 1. Molar composition of natural gas [%]²¹.

Components	Formula	Typical	Extreme
Methane	CH ₄	80-95	50-95
Ethane	C ₂ H ₆	2-5	2-20
Propane	C ₃ H ₈	1-3	1-12
Butane	C ₄ H ₁₀	0-1	0-4
Pentane+	C ₅ +	0-1	0-1
Carbon dioxide	CO ₂	1-5	0-99
Nitrogen	N ₂	1-5	0-70
Hydrogen sulfide	H ₂ S	0-2	0-6
Oxygen	O ₂	0	0-0.2
Helium	He	0-0.1	0-1
Other inert gases		traces	

Table 2. Shale gas composition for different shale plays in USA [mol %]¹⁸.

Well No.	C ₁	C ₂	C ₃	CO ₂	N ₂
Barnett shale gas					
1	80.3	8.1	2.3	1.4	7.9
2	81.2	11.8	5.2	0.3	1.5
3	91.8	4.4	0.4	2.3	1.1
4	93.7	2.6	0.0	2.7	1.0
Average	86.8	6.7	2.0	1.7	2.9
Marcellus shale gas					
1	79.4	16.1	4.0	0.1	0.4
2	82.1	14.0	3.5	0.1	0.3
3	83.8	12.0	3.0	0.9	0.3
4	95.5	3.0	1.0	0.3	0.2
Average	85.2	11.3	2.9	0.4	0.3
Fayetteville shale gas					
Average	97.3	1.0	0.0	1.0	0.7
New Albany shale gas					
1	87.7	1.7	2.5	8.1	
2	88.0	0.8	0.8	10.4	
3	91.0	1.0	0.6	7.4	
4	92.8	1.0	0.6	5.6	
Average	89.9	1.1	1.1	7.9	
Antrim shale gas					
1	27.5	3.5	1.0	3.0	65.0
2	57.3	4.9	1.9	0.0	35.9
3	77.5	4.0	0.9	3.3	14.3
4	85.6	4.3	0.4	9.0	0.7
Average	62.0	4.2	1.1	3.8	29.0
Haynesville shale gas					
Average	95.0	0.1	0.0	4.8	0.1

Table 3. Conversion technologies included in the model.

No.	Process description	Reference
1	Benzene via direct methane aromatization (DMA)	6
2	Syngas ($H_2:CO = 2:1$) via auto-thermal reforming (ATR)	7
3	Syngas ($H_2:CO = 2:1$) via combined reforming (CR)	7
4	Syngas ($H_2:CO = 2:1$) via dry reforming (DR)	22,23
5	Syngas ($H_2:CO = 2:1$) via partial oxidation (POX)	7
6	Syngas ($H_2:CO = 2:1$) via steam methane reforming (SMR)	7
7	Methanol via syngas ($H_2:CO = 2:1$)	7
8	DME via syngas ($H_2:CO = 2:1$)	24
9	DME via methanol dehydration (MD)	25,26
10	Ethylene via methane cracking (MC)	8,27
11	Ethylene via oxidative coupling of methane (OCM)	28
12	Ethylene via non-oxidative coupling of methane (NOCM)	29
13	Ethylene via methane to olefins (MTO)	28
14	Ethylene via ethane cracking (EC) with external refrigerant	8,27
15	Ethylene via ethane cracking (EC) with refrigerant co-produced	30
16	Ethylene via ethane cracking (EC) and propane dehydrogenation (PD)	31
17	Ethylene via ethane-propane mixture (EPM) cracking ($C_2:C_3 = 2.21:1$)	31
18	Ethylene via propane cracking (PC)	30
19	Propylene via propane dehydrogenation (PD)	32
20	Butadiene via dimerization of ethylene (DOE) at 1273 K	33
21	Butadiene via dimerization of ethylene (DOE) at 2773 K	33
22	Ammonia via Haber-Bosch (HB) process	34
23	Urea (prilled) from ammonia ($NH_3: CO_2 = 3.5:1$)	35

Table 4. Input coefficient, $\alpha_{i,j}^{in}$ [kg/kg of product].

Process*	1	2	3	4	5	6	7	8	9
C ₁	2.007	0.585	0.502	0.255	0.569	0.500			
CO ₂				0.682					
O ₂		0.785	0.466		0.720				
H ₂				0.065					
Syngas							1.379	2.803	
CO							0.019		
Methanol									1.491
H ₂ O		0.376	0.807			1.621			
Process*	10	11	12	13	14	15	16	17	18
C ₁	4.032	7.040	7.596						
C ₂					1.188	1.290	1.207	1.089	
C ₃							0.814	0.489	2.380
O ₂	5.228	6.662							
Methanol				4.665					
NaOH					0.002		0.448	0.485	
NMP	0.006								
H ₂ O		0.057					20.000	8.800	
Process*	19	20	21	22	23				
C ₃	1.168								
CO ₂					0.465				
N ₂				1.313					
H ₂				0.288					
Ethylene		2.583	1.733						
NH ₃					0.628				
H ₂ O		3.318	6.610						

* Process numbers refer to Table 3.

Table 5. Output coefficient, $\alpha_{i,j}^{out}$ [kg/kg of product].

Process*	1	2	3	4	5	6	7	8	9
C ₁	0.054								
CO ₂		0.226			0.181			0.963	0.001
H ₂	0.197					0.060			
Benzene	1.000								
Syngas		1.000	1.000	1.000	1.000	1.000	0.390		
Methanol							1.000		
DME								1.000	1.000
Naphtha	0.299								
Coke	0.281								
Tail							0.007	0.829	
H ₂ O		0.519	0.774		0.107	1.060			0.481
Process*	10	11	12	13	14	15	16	17	18
C ₁						0.110			0.650
C ₂				0.018					
C ₃						0.040			
C ₄				0.200		0.040	0.105	0.067	0.100
CO ₂		4.261		0.005					
H ₂			1.682		0.057	0.080	0.142	0.086	0.050
Benzene			1.312						
LPG				0.081	0.038				
Naphtha			1.594						
Ethylene	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Propylene				0.590			0.697	0.227	0.400
Coke				0.062					
Tail	0.804	4.863	0.285	0.040	0.038				0.100
H ₂ O		3.633		2.622					
Propadiene	0.038								
Pygas						0.020			0.160
C ₅ +				0.044				0.013	
Process*	19	20	21	22	23				
H ₂	0.043		0.037						
LPG	0.004								
Ethylene		1.450	0.697						
Butadiene		1.000	1.000						
Propylene	1.000								
NH ₃				1.000					

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UAN				0.111
Urea				1.000
Tail	0.091	0.134		
H ₂ O		3.317	6.608	0.300

* Process numbers refer to Table 3.

** When molar composition stream is lower than 94%, it is considerate tail.

*** C₃ and C₄ mix are considerate as LPG.

Table 6. Utility consumption [GJ/1000 kg of product].

Process*	Cooling, available at					
	30 °C	5 °C	-20 °C	-50 °C	-100 °C	-150 °C
1	21.395					
2	6.766					
3	8.079					
4	3.345					
5	4.700					
6	8.673					
7	4.722				0.009	
8	6.559				5.016	
9	2.941					
10	48.641		1.694		0.027	
11	102.770		1.285		10.545	
12	35.594					
13	11.277	2.837				
14	9.367	0.157	0.920	2.894	0.090	0.056
15	25.021**					
16	11.897					
17	5.276					
18	25.021**					
19	17.696					
20	12.921				1.820	
21	26.082					2.361
22	7.962					
23	9.683**					
Process*	Heating, available as			Electricity		
	LP	HP	Fuel			
1		3.352	12.962		5.299	
2	0.028	1.097	0.637			
3	0.028	2.556	4.967			
4		0.296	5.339		1.557	
5	0.028	0.488				
6	0.046	4.730	11.741			
7	0.096				0.589	
8	4.448				0.556	
9	1.153	1.972			0.006	
10	5.878		17.388		19.205	
11	9.956	1.093			23.681	
12			90.350		13.632	
13	9.686				0.187	
14	5.138		15.660		5.587	
15			21.000		0.504	
16			27.176			
17			13.144			

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18			24.600	0.648
19	11.735		7.874	1.760
20	2.452***		7.376	4.413
21	5.417***		11.701	4.967
22		5.971	0.910	
23		0.847		0.458

* Process numbers refer to Table 3.

** Assumed as saturated liquid at 29 °C

*** Assumed as saturated vapor and full condensation at 2 bar.

Table 7. Base fixed cost investment (FCI) [Adjusted to MM\$ 2019]

Process*	FCI**	Capacity***	Reference
1	1923.0	7000	6
2	510.8	6100	7,36
3	412.4	6100	7,36
4	346.0	6100	36
5	652.0	6100	7,36
6	432.9	6100	7,36
7	416.6	4400	2,7,36
8	403.4	3600	37,38
9	223.9	3600	37,38
10	822.1	7100	2,8
11	772.8	7100	2,28
12	3710.2	7100	2,29
13	772.1	7100	2,28
14	1858.9	7100	2,8
15	1858.9	7100	2,8
16	1757.4	7100	2,31
17	1374.3	7100	2,31
18	2137.8	7100	8,39
19	1019.1	3800	32
20	324.6	1000	33
21	470.9	1000	33
22	238.9	3000	34,40
23	17.0	3500	34,41,42

* Process numbers refer to Table 3.

** FCI was taken as 85% of the total capital investment.

*** T of main product/d

**** Syngas capacity plants were estimated from mass balance for methanol production.

Table 8. Cost of chemicals [\$/T].

Chemical	Cost	Reference	Chemical	Cost	Reference
C ₁	178.2	19	Ethylene	1041.0	4
C ₂	264.3	19	Butadiene	1176.0	43
C ₃	463.6	19	Propylene	950.0	32
C ₄	472.3	19	NH ₃	552.0	37
CO ₂	43.1	44	NaOH	490.0	43
N ₂	525.0	45	NMP	2682.0	43
O ₂	155.0	44	UAN	200.0	46
H ₂	2000.0	6,31	Urea (prilled)	243.0	43
Benzene	842.0	43	Coke	157.0	43
Syngas	315.6	47	Tail	89.1	*
CO	75.0	47	H ₂ O	0.2	31
Methanol	432.0	48	Propadiene	3000.0	49
DME	598.4	48	Pygas	110.0	50
Naphtha	919.3	51	C ₅₊	660.2	19
LPG	476.2	52			

* Tail gas cost was considered half of methane price.

Table 9. Utility costs [\$/GJ].

Utility	Cost	Reference	Utility	Cost	Reference
Cooling, at 30°C	0.95	33	Cooling, at -150°C	18.97	8
Cooling, at 5°C	4.43	53	Heating, LP	14.05	53
Cooling, at -20°C	7.89	53	Heating, HP	17.70	53
Cooling, at -50°C	11.38	33	Heating, fuel	11.10	53
Cooling, at -100°C	13.11	53	Power	29.11	37

Table 10. Demands estimated for 2021 used as initial bound in production network.

Chemical	Demand [MMT/y]	Reference	Increase [%/y]	Reference
Benzene	1.89	54	2.90	55
Methanol	3.60	54	7.96	2
DME	0.15	56,57	8.00	57
Ethylene	0.52	54	7.69	2
Butadiene	0.04	54	3.95	2
Propylene	0.22	54	9.24	2
Ammonia	2.63	54	3.50	58
Urea	2.86	54	2.00	59

Table 11. Total utility consumption by plant [MMGJ].

Plant	Cooling	Heating	Electricity
Benzene	251.2	191.5	62.2
Syngas	296.7	565.0	0.0
Methanol	171.7	3.5	21.4
Ethylene	256.0	649.8	98.0
Propylene	51.6	57.2	5.1
Butadiene	6.9	4.6	2.1
Total	1,034.2	1,471.7	188.8

Figure 1. Chemicals considered in the model and their transformation technologies.

Figure 2. Overall representation of the superstructure for the shale gas industrial park.

Figure 3. Compact representation of mass balances for the network.

Fig. 4. Selection of production technologies.

Fig. 5. Production network by plant for the multi-period development plan [ED=exogenous demand; CP=plant capacity; IP=internal production].

Fig. 6. NPV variation with time for the production network.

Fig. 7. Water nexus.

Fig. 8. Breakdown of utility requirements.

Fig. 9. Effect of shale gas cost on plant capacity in the multi-period production complex.

Fig. 10. Results from the sensitivity analysis against changes in shale gas prices. (a) Yearly NPV as a function of shale gas prices. (b) Accumulated NPV for the 10-year period as a function of shale gas prices.