Integrating biofuels in refinery optimization models

Have a full economic representation without significantly increasing complexity

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Representing biofuels efficiently in refinery optimization models is a new challenge to modelers, mainly due to the varying legislation options and the valorization of a virtual product, the biocertificate. This is even more complex because different national legislations are using different mechanisms across various countries, forcing different economic approaches. This article proposes a simple, yet efficient, way to model these biofuels to have a full economic representation without having to considerably increase complexity of the models. The “trick” is to build virtual process units pretreating biocomponents prior to blending, separating the biocertificate valorization from the physical blending component.

Biofuel types. Today’s main biofuels fall into two categories:
• Biodiesel produced out of vegetable oils and similar feedstocks, known as FAME. The feedstocks are mainly rapeseed or canola oil in the EU, soybean or palm oil are among the favorites elsewhere.
• Biogasoline, i.e., ethanol and added either neat or reacted with isobutylene to bio-ETBE. Both FAME and ethanol are limited in “regular” motor fuels: up to 5 vol% FAME in diesel according to the European EN590 specification, up to 7 vol% in France in 2008 and up to 5% ethanol in gasoline according to the European EN228 specification, and up to 10% in the US and most of the world. Bio-ETBE is limited to 15% or by the gasoline maximum oxygen content. New biofuels are emerging on the market, especially on the biodiesel side:
• Hydrotreated vegetable oils—in special units or using existing refinery hydrotreating units. Qualities vary, but they have in common very high paraffinic content, low gravity and high cetane number.
• Biomass-to-liquid (BTL) diesel, with similar qualities but produced out of cellulosic biomass. This process only exists at the pilot level so far, even though Choren opened the first significantly sized unit.

Why integrate biofuels? I will not try to enter the political arguments about promoting biofuels since this is a decision for political leaders. In many countries, arguments for developing biofuels include greenhouse gas reductions, energy independence and support to the local farming industry. The main driver to incorporate biofuels is because legislation dictates so. This is also part of the problem: Legislations are as numerous as countries legislating, when not regions or states.

Specifics of national legislations. Types of legislation promoting biofuels can be roughly divided into two categories:
• Mandate. Companies marketing diesel and gasoline are required to sell a given percentage of biofuels. This percentage can be based on volume or energy content, as it can be on “motor fuels” globally (so-called “flexible mandates”) as well as on gasoline and diesel separately, or a combination of both.
• Tax breaks. For each liter of biofuel produced / sold, companies get a tax incentive, usually a discount on the duty. To protect themselves against the tax incentive cost spinning out of control, some countries have set quotas globally or by awarding volumes to given (often national) producers. Normally, the volumes to comply with mandates or to claim tax incentives are measured at the duty point and are yearly numbers; there is no need to follow up on every liter of biofuel and its percentage in every liter of fuel sold, Austria being a major exception.

Modelization options. Option 1. Include a “biofuels specification” in the product specification tables. Biofuels in this option is just a blending component like any other, with a quality known as “biocontent”. Other blending components have 0% biocontent. An example of such a set-up is shown in Tables 1, 2 and 3. Pros:
It is a simple option. You need to define:
• A “biofuels content quality” in the property table. Ethanol or FAME will get 100%, ETBE typically 47%
• A “min spec” for that quality in the specification table. The biofuels prices will be as actually paid.
Blending is generally done by volume: Every percentage needs to be in volume as well.

Cons:
- This option does not allow optimizing biofuels compliance between gasoline and diesel when the mandates are flexible.
- There is no calculation of the biofuels coverage cost. This is especially limiting when a certificate market is established.

Therefore, this option is best used when a biofuels blending strategy is calculated offline using another tool. This forces an analyst to use biofuels-specific tools, making sure the biobalance is covered appropriately. Even though this will do the job, it will be time-consuming for the analyst, requiring a specific tool, and will not link fuels production with its economic biofuels element.

**Option 2. Force biofuels volumes to be blended.** This is even easier than the previous option: calculate by hand how much biofuels you need to blend and force the model to buy and use this volume (fixing min and max volumes).

**Pros:**
- Easy and quick to implement.

**Cons:**
- All the above. There is no optimization at all; biofuels are merely represented to be included in the mass-balances. You may even need to force the material balance to close if prices are well above their “fossil fuel” destination.

Now, in fairness, what is the point of representing biofuels in an economic model if no economic conclusion can be derived from it? This is the reason why a more complete, accurate yet easy-to-implement solution is proposed in option 3.

**Option 3. Build certificate units.** The way to represent biofuels’ true economic value is to use the fact that economic model technologies do not need to close the material balance. This allows splitting the biocomponent into its biocertificate value and the physical stream that is routed to the blending.

How is this working? Biofuel components, purchased from the market (“buy” tables) are fed to a virtual process unit, the certificate unit. This virtual unit has a very simple structure: FAME and ethanol as feed stream(s), yielding two products, of which one carries no qualities (a certificate has no gravity, cetane or sulfur). The blend component needs to replicate all relevant qualities from the feed stream, in a simple 1:1 relationship.

Summarized, the certificate unit produces (Fig. 1):
- Blendable biocomponent for 100% yield of the feed
- Certificates, for the appropriate percentage, based on the “bio” quality of the component.

This way, the certificates produced by your model can be sold at market value.

Every destination market needs its specific certificate unit that allows producing separate French gasoline and diesel certificates but to combine diesel and gasoline to produce one motor fuels certificate for the UK, for instance.

Quota volume, as in Belgium, can be lined up via the Belgian certificate unit to Belgian diesel, the Belgian certificate being valued at tax-break value. When the same stream is lined up to the German certificate unit, it will produce a German certificate valued at the German mandate value.

Future sustainability criteria can be accounted for via the biofuels content quality—which is the input fixing the certificate yield.

If your biocomponents from various suppliers have different “bio-%” (e.g., due to different sustainability qualities or biofuels-producing processes), you may allocate each of them its rightful value and easily weigh price vs. sustainability.

**Pros:**
- Accurate economical representation
- Flexible, since many certificates can be produced as required
- All impacts correctly represented.

**Cons:**
- More complex representation than options 1 and 2.

**Word of caution.** All modeling options have their advantages and disadvantages. The main disadvantage of option 3 is if you need to sell into many markets, you may need many certificate units. If prices are close in those markets, you may have a fairly flat optima, potentially leading to suboptimal or nonconverging runs. This is not specific to biofuels introduction, of course, but having more units only reinforces this tendency. To avoid overly complicated optimization runs, you may need to limit the destinations of your biocomponents to sensible outlets only, rather to open all streams to all destinations in a nice-looking, but little-learning, “blue sky” case.

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**TABLE 1. Purchase table**

<table>
<thead>
<tr>
<th>Feed stream</th>
<th>Min.</th>
<th>Max.</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAME</td>
<td>10 kTm</td>
<td>20 kTm</td>
</tr>
<tr>
<td>Ethanol</td>
<td>7 kTm</td>
<td>14 kTm</td>
</tr>
</tbody>
</table>

**TABLE 2. Quality table**

<table>
<thead>
<tr>
<th>Feed stream</th>
<th>SPG</th>
<th>Bio, vol%</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAME</td>
<td>885</td>
<td>...   47</td>
</tr>
<tr>
<td>Ethanol</td>
<td>790</td>
<td>...   100</td>
</tr>
</tbody>
</table>

**TABLE 3. Specification table**

<table>
<thead>
<tr>
<th>Product</th>
<th>Min. SPG</th>
<th>Max. SPG</th>
<th>Bio, vol%</th>
</tr>
</thead>
<tbody>
<tr>
<td>ULSD</td>
<td>820</td>
<td>845</td>
<td>... 4.8</td>
</tr>
<tr>
<td>Premium petrol</td>
<td>720</td>
<td>775</td>
<td>... 4.8</td>
</tr>
</tbody>
</table>

**TABLE 4. Purchase table with amount of purchased biofuels fixed**

<table>
<thead>
<tr>
<th>Feed stream</th>
<th>Min.</th>
<th>Max.</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAME</td>
<td>20 kTm</td>
<td>20 kTm</td>
</tr>
<tr>
<td>Ethanol</td>
<td>14 kTm</td>
<td>14 kTm</td>
</tr>
</tbody>
</table>

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**FIG. 1** Flowsheet of biofuel representation including a “certificate” unit.

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