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Dimethyl Carbonate

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Abstract

Dimethyl carbonate (DMC) is an important industrial chemical. It is used as an intermediate for making polycarbonate, which consumes roughly 50% of its production. Other notable areas of its use include solvents, pesticides, and pharmaceuticals. It is also used as a chemical reagent, particularly for methylation and methoxycarbonylation reactions. It is nontoxic to humans and does not negatively impact the environment, and is also quickly biodegradable, which makes it especially suitable for use as a chemical.

DMC is considered and recommended by some environment and industry experts as a viable choice for use as an oxygenate in transportation fuels, primarily due to its favorable properties needed for fuels—it has about three times more oxygen than methyl tertiary butyl ether (MTBE), and its other plus points as a fuel additive include low vapor pressure, low toxicity, higher boiling point, nonhygroscopic nature, complete miscibility with fuels, and its overall attractive emissions characteristics as a fuel component. If DMC's use as a fuel oxygenate is accepted officially, that would open an enormous market for it. In addition to being environmentally friendly, DMC can also be prepared from natural gas (methanol and CO) and oxygen (air). Hence, unlike MTBE or other solvents, it is not a petroleum derivative. Thus, DMC can potentially also reduce dependence on imported oil.

Traditional synthesis of DMC required toxic and hazardous phosgene as a base material. This disadvantage of the source material prompted researchers to investigate alternate routes for DMC manufacturing that would lower the impact of DMC use on human health and the environment without seriously affecting the economics of production.

This report, therefore, presents technoeconomic assessments of three such nonphosgene-based technologies for DMC production listed below, and the process economics only for the fourth technology listed below:

- Versalis/CB&I's liquid-phase direct methanol oxycarbonylation technology
- Ube's gas-phase indirect methanol oxycarbonylation technology
- Two-step urea-methanol transesterification technology (not commercialized yet)
- Asahi's ethylene carbonate-methanol transesterification technology (only process economics)

The urea-based technology is in the development and refining stage. Different researchers and developers are trying to improve the overall yield of DMC in the process. This technology is now owned by CB&I, which has currently stopped further work on it.

Versalis/CB&I's methyl oxycarbonylation technology is based on a single-step, liquid-phase, cuprous chloride-catalyzed process, which was originally developed by Polymeri/EniChem. Versalis was created as a subsidiary or rename for Polymeri/EniChem. CB&I is the partner in licensing and engineering of contracts. Our evaluation of the technology is based on a single-train plant, producing about 25,000 metric tons per annum (MTPA) of DMC. The chemistry of the process is simple, but small amounts of corrosive by-products are generated that necessitate the use of glass-lined material for certain equipment. The overall

yield of DMC, according to IHS estimates, is 91.9% (based on methanol). Versalis/CB&I primarily produces DMC for the merchandise market.

Ube's methanol oxycarbonylation technology is based on a two-step (or indirect), gas-phase, palladium–copper chloride–catalyzed process. This process has a somewhat more complex chemistry. In the first-phase, methyl nitrite (MN) is carbonylated producing DMC and nitric oxide (NO) in a fixed-bed reactor. In the second step, NO reacts noncatalytically with oxygen and methanol, producing MN and water. This MN is recycled into the first step. Hence, basically only CO, O₂, and methanol are consumed in the process. Overall yield of DMC is equivalent to 92.5% (based on methanol). Ube's process, according to IHS estimates, is somewhat costlier than Versalis/CB&I's process in terms of capital cost. However, the production cost of DMC for the two processes is pretty close, mainly due to the fact that the Ube process produces dimethyl oxalate also as a by-product, which improves the economy of the process. Ube produces DMC primarily to sell it in the merchandise market.

Our third technology analysis is for DMC production by a urea transesterification process using methanol. Since this process is not commercialized yet, a generic-type analysis is presented, based on the data given in the patents of Catalytic Distillation Technologies (CDTECH). The conversion of urea-methanol to DMC is carried out in two steps—first, the urea is converted to methyl carbamate (MC) by reacting with methanol at relatively low temperatures (e.g., 100°C in the presence of a catalyst, or 150°C without catalyst); then, the carbamate is further reacted with methanol at 180–190°C in the presence of a catalyst, producing DMC.

Contents

1	Introduction	8
2	Summary	10
	Overview	10
	Commercial	10
	Technical	12
	Technologies	14
	Versalis/CB&I liquid-phase technology	14
	Ube gas-phase technology	15
	Urea methanolysis technology	16
	Cost estimates	17
	Process economics scope	17
	Methanol oxycarbonylation processes (Versalis/CB&I technology versus Ube technology)	18
3	Market status	23
4	Technical review	28
	DMC production route alternatives	28
	Synthesis of DMC by phosgene methanolysis	28
	Synthesis of DMC by oxidative carbonylation of methanol	29
	Liquid-phase oxidative carbonylation of methanol	29
	Gas-phase oxidative carbonylation of methanol (direct method)	31
	Gas-phase oxidative carbonylation of methanol (indirect method)	33
	Dimethyl carbonate from transesterification of ethylene carbonate	34
	Dimethyl carbonate from methanolysis of urea	37
5	Dimethyl carbonate production by Versalis/CB&I process	46
	Process economics scope	46
	Process description	47
	Process discussion	52
	Feedstock	52
	By-product organic compounds removal	52
	Process streams	52
	Materials of construction	53
	Miscellaneous plant sections	53
	Cost estimates	55
	Fixed-capital costs	55
	Production costs	56
6	Dimethyl carbonate production by Ube indirect gas-phase process	60
	Process economics scope	60
	Process description	61
	Process discussion	65
	Feedstock	65
	Products separation	66
	Materials of construction	66
	Miscellaneous plant sections	66
	Cost estimates	69
	Fixed-capital costs	69
	Production costs	69

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7	Dimethyl carbonate production by Catalytic Distillation Technologies	73
	Process economics scope	73
	Process description	74
	Process discussion	78
	Feedstock	78
	Reactive distillation	78
	Materials of construction	78
	Miscellaneous plant sections	79
	Cost estimates	81
	Fixed-capital costs	81
	Production costs	82
	Appendix A—Patent summaries	86
	Appendix B—Design and cost basis	100
	Design conditions	101
	Cost bases	101
	Capital investment	101
	Production costs	102
	Effect of operating level on production costs	102
	Appendix C—Cited references	104
	Appendix D—Process flow diagrams	106

Tables

Table 2.1	Global DMC production forecast by global regions (2017–22)	11
Table 2.2	Methanol oxycarbonate technologies—Total capital investment	19
Table 2.3	Methanol oxycarbonate technologies—Production costs	20
Table 2.4	Urea and ethylene oxide transesterification technologies—Total capital investment	21
Table 2.5	Urea and ethylene oxide transesterification technologies—Production costs	22
Table 3.1	Global DMC production forecast by global regions (2017–22)	24
Table 3.2	Global DMC production forecast by application type (2017–22)	25
Table 3.3	Global DMC consumption forecast for different regions of the world (2017–22)	26
Table 4.1	Catalyst metal effect on DMC yield	30
Table 4.2	Effect of catalyst anions on DMC yield	30
Table 4.3	Effect of catalyst support on DMC yield	30
Table 4.4	Effect of copper catalyst promoters on DMC yield	31
Table 4.5	Effect of ratio of the copper catalyst promoters on DMC yield	31
Table 4.6	Performance of zinc/yttrium catalysts in DMC synthesis	37
Table 4.7	Performance of lanthanum catalysts in DMC synthesis ^a	38
Table 4.8	Effect of different catalysts on MC and DMC yields ^a	41
Table 4.9	Performance of solid-base catalysts in DMC synthesis	43
Table 4.10	Effect of catalysts on MC and DMC yields ^a	43
Table 5.1	DMC production by Versalis/CB&I process—Design bases and assumptions	49
Table 5.2	DMC production by Versalis/ CB&I process—Main stream flows	49
Table 5.3	DMC production by Versalis/CB&I process—Major equipment	54
Table 5.4	DMC production by Versalis/CB&I process—Utilities summary	55
Table 5.5	DMC production by Versalis/CB&I process—Total capital investment	57
Table 5.6	DMC production by Versalis/CB&I process—Production costs	58
Table 6.1	DMC production by Ube indirect gas-phase process—Design bases and assumptions	63
Table 6.2	DMC production by Ube indirect gas-phase process—Main stream flows	64
Table 6.3	DMC production by Ube indirect gas-phase process—Major equipment	67
Table 6.4	DMC production by Ube indirect gas-phase process—Utilities summary	68
Table 6.5	DMC production by Ube indirect gas-phase process—Total capital investment	70

Table 6.6 DMC production by Ube indirect gas-phase process—Production costs	71
Table 7.1 DMC production by CDTECH—Design bases and assumptions	76
Table 7.2 DMC production by CDTECH—Main stream flows	76
Table 7.3 DMC production waste streams	78
Table 7.4 DMC by CDTECH—Utilities summary	79
Table 7.5 DMC by CDTECH—Major equipment	80
Table 7.6 DMC by CDTECH—Total capital investment	83
Table 7.7 DMC by CDTECH—Production costs	84

Figures

Figure 2.1 World consumption of DMC in 2016	10
Figure 2.2 Global DMC production share forecast by global regions (2017–22)	11
Figure 2.3 Global DMC production share forecast by application type (2017–22)	12
Figure 3.1 World consumption of DMC in 2016	23
Figure 3.2 Global DMC production share forecast by global regions (2017–22)	24
Figure 3.3 Global DMC production share forecast by application type (2017–22)	25
Figure 3.4 Global DMC production share forecast from different processes (2017–22)	26
Figure 3.5 Global DMC consumption share forecast by global regions (2017–22)	27
Figure 3.6 Global DMC consumption share forecast by applications (2017–22)	27
Figure 4.1 Effect of reaction temperature on DMC synthesis	39
Figure 4.2 Effect of reaction time on DMC synthesis	39
Figure 4.3 Effect of reaction temperature on DMC yield in catalytic distillation reactor	44
Figure 4.4 Effect of urea LHSV on DMC yield in catalytic distillation reactor	45
Figure 5.1 DMC production by Versalis/Lummus process	107
Figure 6.1 DMC production by Ube indirect gas-phase process	108
Figure 7.1 DMC production by CDTECH—Section 100 (sheet 1 of 2)	109
Figure 7.1 DMC production by CDTECH—Section 200 (sheet 2 of 2)	110

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