Electronic Supplementary Material (ESI) for Energy & Environmental Science.


**Supplementary Material.**

# From fossil to green chemicals: Sustainable pathways and new carbon feedstocks for the global chemical industry

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**Table of Contents**

# 1. Chemical Demand Modelling

**Table S1.** Distribution of primary chemical demands among downstream chemicals modelled according to Horton.[1]

| **Distribution of Ethylene Demands** | |
|---|---|
| Polyethylene | 61% |
| Ethylene oxide | 15% |
| Ethylene dichloride | 9% |
| Styrene | 5% |
| Others | 10% |
| **Distribution of Propylene Demands** | |
| Polypropylene | 60% |
| Propylene Oxide | 7% |
| Acrylonitrile | 10% |
| Cumene | 4% |
| Isopropanol | 1% |
| Others | 18% |
| **Distribution of Benzene Demands** | |
| Styrene | 49% |
| Cumene | 20% |
| Others | 31% |
| **Distribution of Mixed Xylenes Demands** | |
| Para-xylenes | 93% |
| Others | 7% |

**Table S2.** Share of final chemicals to plastic production according to global chemical flows from Levi and Cullen[2]. Final chemicals not listed here are assumed to not be used for any plastic production.

| **Chemical-to-plastic** | **Share** |
|---|---|
| Polyethylene-to-plastic | 100% |
| Vinyl chloride-to-plastic | 100% |
| Other ethylene-to-plastic | 100% |
| Polypropylene-to-plastic | 100% |
| Terephthalic acid-to-plastic | 33.1% |
| Ethylene Glycol-to-plastic | 33% |
| Styrene-to-plastic | 57% |
| Other Benzene-to-plastics | 11% |
| Toluene-to-plastics | 7% |

**Table S3.** Plastic collection CAGR by region from 1990-2019, collection-to-recycling ratio in 2019, and collection-to-recycling growth rate by OECD region.

| | Plastic collection CAGR (1990-2019) | Collection-to-recycling ratio | Collection-to-recycling CAGR BAU (2000-2019) | Collection-to-recycling growth rate p.a. NZE 2050 | Collection-to-recycling growth rate p.a. NZE 2040 | Collection-to-recycling growth rate p.a. NZE 2060 |
|---|---|---|---|---|---|---|
| United States | 4% | 50.7% | 0.2% | 16% | 25% | 12% |
| Canada | 5% | 51.1% | 0.2% | 16% | 24% | 12% |
| Other OECD America | 5% | 70.3% | 0.1% | 10% | 15% | 7% |
| OECD Europe | 12% | 56.3% | 0.4% | 15% | 22% | 11% |
| OECD Non-EU | 12% | 54.4% | 0.2% | 15% | 23% | 11% |
| OECD Asia | 12% | 56.5% | 0.3% | 15% | 22% | 11% |
| OECD Oceania | 5% | 59.9% | 0.1% | 13% | 20% | 10% |
| Non-OECD Latin America | 5% | 70.5% | 0.01% | 10% | 15% | 7% |
| Non-OECD Other EU | 13% | 59.0% | 0.1% | 14% | 20% | 10% |
| Non-OECD Eurasia | 5% | 58.2% | 0.1% | 14% | 21% | 10% |
| MENA | 5% | 66.6% | 0.003% | 11% | 17% | 8% |
| Non-OECD Other Africa | 5% | 70.0% | 0.1% | 10% | 15% | 8% |
| Other Non-OECD Asia | 5% | 61.8% | 0.1% | 13% | 19% | 10% |
| China | 12% | 63.3% | 0.03% | 12% | 18% | 9% |
| India | 12% | 67.5% | 0.1% | 11% | 16% | 8% |
| Total | 7% | 60.2% | 0.3 % | 13% | 20% | 10% |

**Table S4.** Recycling rate by region in the BAU scenario.

| **Recycling rate by region** | 2020 | 2030 | 2040 | 2050 | 2060 | 2070 | 2080 | 2090 | 2100 |
|---|---|---|---|---|---|---|---|---|---|
| United States | 4.7% | 6.3% | 8.4% | 11.3% | 15.1% | 20.2% | 27.1% | 34.8% | 35.4% |
| Canada | 6.8% | 9.1% | 12.2% | 16.4% | 22.0% | 29.4% | 34.4% | 35.0% | 35.7% |
| Other OECD America | 10.7% | 14.3% | 19.2% | 25.7% | 34.4% | 46.1% | 47.3% | 48.2% | 49.2% |
| OECD Europe | 16.0% | 21.4% | 28.7% | 35.8% | 36.5% | 37.2% | 37.9% | 38.7% | 39.4% |
| OECD Non-EU | 8.6% | 11.6% | 15.5% | 20.8% | 27.9% | 35.9% | 36.6% | 37.3% | 38.0% |
| OECD Asia | 13.4% | 18.0% | 24.1% | 32.3% | 36.6% | 37.3% | 38.0% | 38.7% | 39.5% |
| OECD Oceania | 7.2% | 9.7% | 13.0% | 17.4% | 23.3% | 31.2% | 40.4% | 41.1% | 41.9% |
| Non-OECD Latin America | 10.7% | 14.4% | 19.2% | 25.8% | 34.5% | 46.2% | 47.5% | 48.4% | 49.3% |
| Non-OECD Other EU | 6.8% | 9.2% | 12.3% | 16.5% | 22.1% | 29.6% | 39.6% | 40.5% | 41.3% |
| Non-OECD Eurasia | 5.0% | 6.7% | 9.0% | 12.0% | 16.1% | 21.5% | 28.9% | 38.7% | 40.7% |
| MENA | 5.7% | 7.6% | 10.2% | 13.7% | 18.4% | 24.6% | 33.0% | 44.2% | 46.6% |
| Non-OECD Other Africa | 6.0% | 8.0% | 10.8% | 14.4% | 19.3% | 25.9% | 34.6% | 46.4% | 48.9% |
| Other Non-OECD Asia | 9.4% | 12.6% | 16.9% | 22.6% | 30.3% | 40.6% | 41.6% | 42.4% | 43.2% |
| China | 14.4% | 19.3% | 25.8% | 34.6% | 41.1% | 41.8% | 42.6% | 43.4% | 44.3% |
| India | 15.0% | 20.1% | 26.9% | 36.1% | 43.7% | 44.6% | 45.4% | 46.3% | 47.2% |
| Total | 10.0% | 13.4% | 18.0% | 24.0% | 32.2% | 39.7% | 40.5% | 41.3% | 42.1% |

**Table S5.** Recycling rate by region in the NZE 2050 scenario.

| **Recycling rate by region** | 2020 | 2030 | 2040 | 2050 | 2060 | 2070 | 2080 | 2090 | 2100 |
|---|---|---|---|---|---|---|---|---|---|
| United States | 4.7% | 10.3% | 45.1% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Canada | 6.8% | 12.7% | 45.6% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Other OECD America | 10.7% | 16.5% | 49.2% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Europe | 16.0% | 22.8% | 48.0% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Non-EU | 8.6% | 14.7% | 46.4% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Asia | 13.4% | 19.9% | 47.6% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Oceania | 7.2% | 13.0% | 47.0% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Latin America | 10.7% | 16.5% | 49.3% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Other EU | 6.8% | 12.6% | 46.8% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Eurasia | 5.0% | 10.6% | 46.4% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| MENA | 5.7% | 11.4% | 47.9% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Other Africa | 6.0% | 11.7% | 48.5% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Other Non-OECD Asia | 9.4% | 15.3% | 47.7% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| China | 14.4% | 20.5% | 48.8% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| India | 15.0% | 20.9% | 49.5% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Total | 10.0% | 16.0% | 47.5% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |

**Table S6.** Recycling rate by region in the NZE 2040 scenario.

| **Recycling rate by region** | 2020 | 2030 | 2040 | 2050 | 2060 | 2070 | 2080 | 2090 | 2100 |
|---|---|---|---|---|---|---|---|---|---|
| United States | 4.7% | 26.1% | 59.1% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Canada | 6.8% | 27.7% | 59.2% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Other OECD America | 10.7% | 32.0% | 59.2% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Europe | 16.0% | 34.5% | 59.4% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Non-EU | 8.6% | 29.3% | 59.2% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Asia | 13.4% | 32.8% | 59.3% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Oceania | 7.2% | 28.8% | 59.1% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Latin America | 10.7% | 32.0% | 59.2% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Other EU | 6.8% | 28.5% | 59.1% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Eurasia | 5.0% | 27.1% | 59.1% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| MENA | 5.7% | 28.6% | 59.1% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Other Africa | 6.0% | 29.1% | 59.1% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Other Non-OECD Asia | 9.4% | 30.4% | 59.2% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| China | 14.4% | 33.8% | 59.3% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| India | 15.0% | 34.4% | 59.3% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |
| Total | 10.0% | 30.7% | 59.2% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% | 60.0% |

**Table S7.** Recycling rate by region in the NZE 2060 scenario.

| **Recycling rate by region** | 2020 | 2030 | 2040 | 2050 | 2060 | 2070 | 2080 | 2090 | 2100 |
|---|---|---|---|---|---|---|---|---|---|
| United States | 4.7% | 5.9% | 11.5% | 47.3% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| Canada | 6.8% | 8.5% | 14.3% | 47.8% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| Other OECD America | 10.7% | 11.9% | 17.5% | 50.6% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Europe | 16.0% | 19.1% | 25.1% | 50.1% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Non-EU | 8.6% | 10.5% | 16.3% | 48.5% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Asia | 13.4% | 16.1% | 22.0% | 49.6% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| OECD Oceania | 7.2% | 8.5% | 14.2% | 48.8% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Latin America | 10.7% | 11.9% | 17.5% | 50.6% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Other EU | 6.8% | 8.1% | 13.8% | 48.7% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Eurasia | 5.0% | 6.0% | 11.6% | 48.2% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| MENA | 5.7% | 6.5% | 12.2% | 49.4% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| Non-OECD Other Africa | 6.0% | 6.7% | 12.5% | 49.8% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| Other Non-OECD Asia | 9.4% | 10.9% | 16.6% | 49.4% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| China | 14.4% | 16.5% | 22.2% | 50.5% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| India | 15.0% | 16.8% | 22.4% | 51.0% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |
| Total | 10.0% | 11.7% | 17.4% | 49.4% | 59.9% | 60.0% | 60.0% | 60.0% | 60.0% |

**Table S8.** Plastic waste incineration CAGR by region from 1990-2019, collection-to-recycling ratio in 2019, and collection-to-recycling growth rate by OECD region.

| | **Plastic incineration CAGR (1990-2019)** | **Plastic incineration-growth rate p.a. NZE 2050** | **Collection-to-recycling growth rate p.a. NZE 2040** | **Collection-to-recycling growth rate p.a. NZE 2060** |
|---|---|---|---|---|
| United States | 1% | 7% | 10% | 5% |
| Canada | 1% | 12% | 18% | 9% |
| Other OECD America | 1% | 13% | 20% | 10% |
| OECD Europe | 11% | -1% | -2% | -1% |
| OECD Non-EU | 5% | 6% | 8% | 4% |
| OECD Asia | 7% | -11% | -16% | -8% |
| OECD Oceania | 1% | 9% | 14% | 7% |
| Non-OECD Latin America | 1% | 13% | 20% | 10% |
| Non-OECD Other EU | 4% | 12% | 19% | 9% |
| Non-OECD Eurasia | 3% | 13% | 19% | 10% |
| MENA | 2% | 13% | 20% | 10% |
| Non-OECD Other Africa | 2% | 13% | 20% | 10% |
| Other Non-OECD Asia | 5% | 12% | 18% | 9% |
| China | 11% | 5% | 8% | 4% |
| India | 8% | 12% | 18% | 9% |
| Total | 4% | 7% | 10% | 5% |

**Table S9.** Plastic incineration rate by region in the BAU scenario.

| **Incineration rate by region** | 2020 | 2030 | 2040 | 2050 | 2060 | 2070 | 2080 | 2090 | 2100 |
|---|---|---|---|---|---|---|---|---|---|
| United States | 19.3% | 21.9% | 24.9% | 28.2% | 32.0% | 36.3% | 41.2% | 46.8% | 53.1% |
| Canada | 4.1% | 4.7% | 5.4% | 6.1% | 6.9% | 7.8% | 8.9% | 10.1% | 11.5% |
| Other OECD America | 0.5% | 0.5% | 0.6% | 0.7% | 0.8% | 0.9% | 1.0% | 1.2% | 1.3% |
| OECD Europe | 49.1% | 50.7% | 57.5% | 64.2% | 63.5% | 62.8% | 62.1% | 61.3% | 60.6% |
| OECD Non-EU | 24.3% | 26.6% | 30.2% | 34.3% | 38.9% | 44.1% | 50.0% | 56.8% | 62.0% |
| OECD Asia | 77.0% | 82.0% | 75.9% | 67.7% | 63.4% | 62.7% | 62.0% | 61.3% | 60.5% |
| OECD Oceania | 11.6% | 13.2% | 15.0% | 17.0% | 19.3% | 21.9% | 24.9% | 28.2% | 32.0% |
| Non-OECD Latin America | 0.6% | 0.6% | 0.7% | 0.8% | 0.9% | 1.1% | 1.2% | 1.4% | 1.6% |
| Non-OECD Other EU | 2.7% | 3.0% | 3.4% | 3.9% | 4.4% | 5.0% | 5.7% | 6.4% | 7.3% |
| Non-OECD Eurasia | 1.1% | 1.2% | 1.3% | 1.5% | 1.7% | 2.0% | 2.2% | 2.5% | 2.9% |
| MENA | 0.6% | 0.7% | 0.8% | 0.9% | 1.0% | 1.2% | 1.3% | 1.5% | 1.7% |
| Non-OECD Other Africa | 0.5% | 0.6% | 0.7% | 0.7% | 0.8% | 1.0% | 1.1% | 1.2% | 1.4% |
| Other Non-OECD Asia | 4.6% | 5.0% | 5.7% | 6.5% | 7.4% | 8.3% | 9.5% | 10.7% | 12.2% |
| China | 26.3% | 27.3% | 31.0% | 35.2% | 39.9% | 45.3% | 51.4% | 56.6% | 55.7% |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| India | 4.5% | 4.8% | 5.4% | 6.2% | 7.0% | 7.9% | 9.0% | 10.2% | 11.6% |
| Total | 19.8% | 21.9% | 24.8% | 28.2% | 32.0% | 36.3% | 41.2% | 46.7% | 53.0% |

**Table S10.** Plastic incineration rate by region in the NZE 2050 scenarios.

| **Incineration rate by region** | 2020 | 2030 | 2040 | 2050 | 2060 | 2070 | 2080 | 2090 | 2100 |
|---|---|---|---|---|---|---|---|---|---|
| United States | 19.3% | 26.3% | 33.3% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| Canada | 4.1% | 11.1% | 18.1% | 25.1% | 32.0% | 39.0% | 40.0% | 40.0% | 40.0% |
| Other OECD America | 0.5% | 7.4% | 14.4% | 21.4% | 28.4% | 35.3% | 40.0% | 40.0% | 40.0% |
| OECD Europe | 49.1% | 56.1% | 52.0% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| OECD Non-EU | 24.3% | 31.2% | 38.2% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| OECD Asia | 77.0% | 80.1% | 52.4% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| OECD Oceania | 11.6% | 18.6% | 25.6% | 32.6% | 39.5% | 40.0% | 40.0% | 40.0% | 40.0% |
| Non-OECD Latin America | 0.6% | 7.5% | 14.5% | 21.5% | 28.5% | 35.4% | 40.0% | 40.0% | 40.0% |
| Non-OECD Other EU | 2.7% | 9.7% | 16.7% | 23.6% | 30.6% | 37.6% | 40.0% | 40.0% | 40.0% |
| Non-OECD Eurasia | 1.1% | 8.0% | 15.0% | 22.0% | 29.0% | 35.9% | 40.0% | 40.0% | 40.0% |
| MENA | 0.6% | 7.6% | 14.6% | 21.5% | 28.5% | 35.5% | 40.0% | 40.0% | 40.0% |
| Non-OECD Other Africa | 0.5% | 7.5% | 14.5% | 21.4% | 28.4% | 35.4% | 40.0% | 40.0% | 40.0% |
| Other Non-OECD Asia | 4.6% | 11.6% | 18.5% | 25.5% | 32.5% | 39.5% | 40.0% | 40.0% | 40.0% |
| China | 26.3% | 33.3% | 40.3% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| India | 4.5% | 11.4% | 18.4% | 25.4% | 32.4% | 39.3% | 40.0% | 40.0% | 40.0% |
| Total | 19.8% | 26.8% | 33.8% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |

**Table S11.** Plastic incineration rate by region in the NZE 2040 scenarios.

| **Incineration rate by region** | 2020 | 2030 | 2040 | 2050 | 2060 | 2070 | 2080 | 2090 | 2100 |
|---|---|---|---|---|---|---|---|---|---|
| United States | 19.3% | 29.8% | 40.2% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| Canada | 4.1% | 14.6% | 25.1% | 35.5% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| Other OECD America | 0.5% | 10.9% | 21.4% | 31.9% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| OECD Europe | 49.1% | 59.6% | 40.6% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| OECD Non-EU | 24.3% | 34.7% | 40.8% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| OECD Asia | 77.0% | 67.2% | 40.7% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| OECD Oceania | 11.6% | 22.1% | 32.6% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| Non-OECD Latin America | 0.6% | 11.0% | 21.5% | 32.0% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| Non-OECD Other EU | 2.7% | 13.2% | 23.6% | 34.1% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| Non-OECD Eurasia | 1.1% | 11.5% | 22.0% | 32.4% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| MENA | 0.6% | 11.1% | 21.5% | 32.0% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| Non-OECD Other Africa | 0.5% | 11.0% | 21.4% | 31.9% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| Other Non-OECD Asia | 4.6% | 15.0% | 25.5% | 36.0% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| China | 26.3% | 36.8% | 40.7% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| India | 4.5% | 14.9% | 25.4% | 35.9% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |
| Total | 19.8% | 30.3% | 40.7% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% | 40.0% |

**Table S12.** Plastic incineration rate by region in the NZE 2060 scenarios.

| **Incineration rate by region** | 2020 | 2030 | 2040 | 2050 | 2060 | 2070 | 2080 | 2090 | 2100 |
|---|---|---|---|---|---|---|---|---|---|
| United States | 19.3% | 24.6% | 29.8% | 35.0% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% |
| Canada | 4.1% | 9.4% | 14.6% | 19.8% | 25.1% | 30.3% | 35.5% | 40.0% | 40.0% |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Other OECD America | 0.5% | 5.7% | 10.9% | 16.2% | 21.4% | 26.6% | 31.9% | 37.1% | 40.0% |
| OECD Europe | 49.1% | 54.3% | 59.6% | 49.9% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% |
| OECD Non-EU | 24.3% | 29.5% | 34.7% | 40.0% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% |
| OECD Asia | 77.0% | 82.2% | 78.0% | 50.4% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% |
| OECD Oceania | 11.6% | 16.9% | 22.1% | 27.3% | 32.6% | 37.8% | 40.0% | 40.0% | 40.0% |
| Non-OECD Latin America | 0.6% | 5.8% | 11.0% | 16.3% | 21.5% | 26.7% | 32.0% | 37.2% | 40.0% |
| Non-OECD Other EU | 2.7% | 8.0% | 13.2% | 18.4% | 23.6% | 28.9% | 34.1% | 39.3% | 40.0% |
| Non-OECD Eurasia | 1.1% | 6.3% | 11.5% | 16.8% | 22.0% | 27.2% | 32.4% | 37.7% | 40.0% |
| MENA | 0.6% | 5.8% | 11.1% | 16.3% | 21.5% | 26.8% | 32.0% | 37.2% | 40.0% |
| Non-OECD Other Africa | 0.5% | 5.7% | 11.0% | 16.2% | 21.4% | 26.7% | 31.9% | 37.1% | 40.0% |
| Other Non-OECD Asia | 4.6% | 9.8% | 15.0% | 20.3% | 25.5% | 30.7% | 36.0% | 40.0% | 40.0% |
| China | 26.3% | 31.6% | 36.8% | 42.0% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% |
| India | 4.5% | 9.7% | 14.9% | 20.2% | 25.4% | 30.6% | 35.9% | 40.0% | 40.0% |
| Total | 19.8% | 25.0% | 30.3% | 35.5% | 40.1% | 40.0% | 40.0% | 40.0% | 40.0% |

Once primary chemical demands were determined, chemical production technologies defined in Sections 1.1 and 1.2 were applied to meet the demand, which were allocated to be satisfied by fossil routes and by e-chemical and bio-chemical routes. For each production technology, there are several co-products, which could be used to reduce the demand for other technologies. The most notable is the steam cracker, which has both propylene and BTX aromatic co-production. Since ethylene is the most widely produced HVC, ethylene demand was first satisfied by the chemical production model. After this step, the propylene demand was re-calculated according to the propylene co-product of steam crackers. The remaining propylene demand was met by catalytic crackers and propane dehydrogenation, the former of which also has a BTX co-product. Fossil BTX demands were then recalculated based on the by-products from steam crackers and catalytic crackers, with the remaining BTX demand being supplied by toluene hydrodealkylation, toluene disproportionation, and naphtha catalytic cracking, representing refinery sourced BTX aromatics. The co-production of the BTX aromatic chemicals led to some overproduction, especially in regions with heavier feedstocks and thus higher shares of BTX aromatic co-products. HVC demands for e-chemical and bio-chemical routes were met by methanol-to-olefins and methanol-to-aromatics, and it was assumed that production ratios of the main products could be controlled by process conditions[2]. Production matrices for each technology are shown in Table S13-Table **S15**.

**Table S13.** Olefin production matrix by feedstock.

| **Feedstock** | | **Unit** | **Naphtha** | **Ethane** | **Propane** | **Butane** | **Gas Oil** | **MTO**[3] |
|---|---|---|---|---|---|---|---|---|
| **Co-products** | **Propylene** | $t/t_{ethylene}$ | 0.53 | 0.04 | 0.4 | 0.43 | 0.58 | 0.63 |
| | **C4 chemicals** | $t/t_{ethylene}$ | 0.34 | 0.04 | 0.1 | 0.26 | 0.36 | 0.18 |
| | **Pygas**[1] | $t/t_{ethylene}$ | 0.75 | 0.02 | 0.16 | 0.18 | 0.50 | 0 |
| | **Hydrogen** | $t/t_{ethylene}$ | 0.05 | 0.08 | 0.05 | 0.04 | 0.03 | 0.01 |
| | **Fuel grade products**[2] | $t/t_{ethylene}$ | 0.63 | 0.11 | 0.75 | 0.60 | 0.46 | 0.06 |

[1] composition of pygas assumed to be 30% benzene, 18.5% toluene, and 8.50% xylenes according to Levi and Cullen[2]

[2] includes C1 chemicals and residual fuel oil

[3] ratio of ethylene and propylene assumed to be adjustable according to Levi and Cullen[2]

**Table S14.** Propylene production matrix by feedstock.

| Feedstock | | Unit | Propane | Refinery Oil |
|---|---|---|---|---|
| **Co-products** | **C4 chemicals** | $t/t_{propylene}$ | 0.04 | 0.8 |
| | **Pygas**[1] | $t/t_{propylene}$ | 0 | 1.3 |
| | **Hydrogen** | $t/t_{propylene}$ | 0.03 | - |
| | **Fuel grade products**[2] | $t/t_{propylene}$ | 0 | 1.3 |

[1] composition of pygas assumed to be 30% benzene, 18.5% toluene, and 8.50% xylenes according to Levi and Cullen[2]

[2] includes C1 chemicals and residual fuel oil

**Table S15.** Aromatic production matrix by feedstock.

| Feedstock | | Unit | Naphtha | MTA[1] |
|---|---|---|---|---|
| **Co-products** | **Benzene** | $t/t_{BTX}$ | 0.14 | 0.084 |
| | **Toluene** | $t/t_{BTX}$ | 0.409 | 0.295 |
| | **Xylenes** | $t/t_{BTX}$ | 0.455 | 0.621 |
| | **Hydrogen** | $t/t_{BTX}$ | 0.203 | - |
| | **Dry gas** | $t/t_{BTX}$ | - | 0.016 |
| | **LPG** | | 0.089 | 1.214 |
| | **Pentane** | | 0.076 | 0.263 |
| | **C6+ alkane** | | 0.290 | - |
| | **C9+** | | 0.322 | 0.176 |

[1] ratio of BTX chemicals assumed to be adjustable as is the case for MTO[2]

## 2. Financial Assumptions

**Table S16.** Financial assumptions by technology. For chemical feedstocks, units are provided per unit energy, and for chemicals produced with feedstock inputs, units are provided per tonne.

| Device | | unit | 2020 | 2030 | 2040 | 2050 | Ref |
|---|---|---|---|---|---|---|---|
| **Solar PV fixed tilted** | capex | €/$kW_p$ | 475 | 306 | 207 | 166 | [3] |
| | $opex_{fix}$ | €/($kW_p$·a) | 8.53 | 6.23 | 4.47 | 3.70 | [3] |
| | lifetime | year | 35 | 40 | 40 | 40 | [4] |
| **Solar PV single-axis tracking** | capex | €/$kW_p$ | 523 | 337 | 228 | 183 | [3] |
| | $opex_{fix}$ | €/($kW_p$·a) | 9.40 | 6.86 | 4.92 | 4.07 | [3] |
| | lifetime | year | | 40 | 40 | 40 | |
| **Wind power (onshore)** | capex | €/$kW_p$ | 1150 | 1000 | 940 | 900 | [4,5] |
| | $opex_{fix}$ | % of capex p.a. | 2 | 2 | 2 | 2 | |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Alkaline water electrolyser** | capex | €/$kW_{H2,LHV}$ | 965 | 489 | 283 | 212 | [6–8] |
| | $opex_{fix}$ | % of capex p.a. | 3.5 | 3.5 | 3.5 | 3.5 | |
| | $opex_{var}$ | €/$kWh_{H2,LHV}$ | 0.0011 | 0.0005 | 0.0005 | 0.0002 | |
| | lifetime | year | 30 | 30 | 30 | 30 | |
| | efficiency, LHV | % | 62.5 | 65.0 | 67.5 | 70.0 | |
| **$H_2$ compressor** | capex | €/$kW_{H2,LHV}$ | 34.32 | 34.32 | 34.32 | 34.32 | [3,9] |
| | $opex_{fix}$ | % of capex p.a. | 4 | 4 | 4 | 4 | [9] |
| | lifetime | year | 30 | 30 | 30 | 30 | |
| **$H_2$ storage** | capex | €/$MWh_{H2,LHV}$ | 1011 | 1006 | 1004 | 1003 | [3,10] |
| | $opex_{fix}$ | % of capex p.a. | 4 | 4 | 4 | 4 | [11] |
| | lifetime | year | 30 | 30 | 30 | 30 | |
| **$NH_3$ Synthesis Plant (including Air Separation Unit, $N_2$ buffer and 30 days of $NH_3$ storage)** | capex | €/$kW_{NH3,LHV}$ | 1053 | 1053 | 1053 | 1053 | [3] |
| | $opex_{fix}$ | % of capex p.a. | 4% | 4% | 4% | 4% | |
| | $opex_{var}$ | €/$MWh_{NH3,LHV}$ | 2.095 | 2.095 | 2.095 | 2.095 | |
| | lifetime | year | 30 | 30 | 30 | 30 | |
| **MeOH Synthesis Unit - incl. 30 days storage** | capex | €/$kW_{MeOH,LHV}$ | 832 | 714 | 613 | 561 | |
| | $opex_{fix}$ | % of capex p.a. | 4 | 4 | 4 | 4 | |
| | $opex_{var}$ | €/$MWh_{MeOH,LHV}$ | 1.9899 | 1.9899 | 1.9899 | 1.9899 | |
| | lifetime | year | 30 | 30 | 30 | 30 | |
| **Coal-to-Methanol** | capex | €/$kW_{MeOH,LHV}$ | 990 | 990 | 990 | 990 | [12] |
| | $opex_{fix}$ | % of capex p.a. | 5 | 5 | 5 | 5 | [12] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Natural Gas-to-Methanol** | capex | €/$kW_{MeOH,LHV}$ | 409 | 409 | 409 | 409 | [12] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [12] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Oil-to-Methanol** | capex | €/$kW_{MeOH,LHV}$ | 390 | 390 | 390 | 390 | [13] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [13] |
| | lifetime | Year | 25 | 25 | 25 | 25 | |
| **Biomass-to-Methanol** | capex | €/$kW_{MeOH,LHV}$ | 1488 | 1488 | 1488 | 1488 | [14] |
| | $opex_{fix}$ | % of capex p.a. | 5 | 5 | 5 | 5 | [14] |
| | lifetime | year | 20 | 20 | 20 | 20 | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **Coal-to-Ammonia** | capex | €/$kW_{NH3,LHV}$ | 3024 | 3024 | 3024 | 3024 | [12] |
| | $opex_{fix}$ | % of capex p.a. | 5 | 5 | 5 | 5 | [12] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Natural Gas-to-Ammonia** | capex | €/$kW_{NH3,LHV}$ | 1258 | 1258 | 1258 | 1258 | [12] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [12] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Oil-to-Ammonia** | capex | €/$kW_{NH3,LHV}$ | 1673 | 1673 | 1673 | 1673 | [12] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [12] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Biomass-to-Ammonia** | capex | €/$kW_{NH3,LHV}$ | 8788 | 8788 | 8788 | 8788 | [12] |
| | $opex_{fix}$ | % of capex p.a. | 5 | 5 | 5 | 5 | [12] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Chlor-alkali electrolyser** | capex | €/t$Cl_2$·a | 1000 | 1000 | 1000 | 1000 | [15] |
| | $opex_{fix}$ | % of capex p.a. | 15 | 15 | 15 | 15 | [15] |
| | lifetime | year | 20 | 20 | 20 | 20 | [16] |
| **Naphtha Steam Cracker** | capex | €/tEthylene·a | 3349 | 3349 | 3349 | 3349 | [13] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [13] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Ethane Steam Cracker** | capex | €/tEthylene·a | 1563 | 1563 | 1563 | 1563 | [13] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [13] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Propane Steam Cracker** | capex | €/tEthylene·a | 2832 | 2832 | 2832 | 2832 | [13] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [13] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Gas Oil Steam Cracker** | capex | €/tEthylene·a | 4321 | 4321 | 4321 | 4321 | [13] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [13] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Butane Steam Cracker** | capex | €/tEthylene·a | 2910 | 2910 | 2910 | 2910 | [13] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [13] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Propane Dehydrogenation** | capex | €/tPropylene·a | 1691 | 1691 | 1691 | 1691 | [13] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [13] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Refinery Oil Catalytic Cracking** | capex | €/tPropylene·a | 5223 | 5223 | 5223 | 5223 | [13] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [13] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Naphtha Catalytic Reforming** | capex | €/tBTX·a | 371 | 371 | 371 | 371 | [17] |
| | $opex_{fix}$ | % of capex p.a. | 4 | 4 | 4 | 4 | |
| | lifetime | year | 20 | 20 | 20 | 20 | |
| **Methanol-to-Olefins** | capex | €/tOlefin·a | 444 | 444 | 444 | 444 | [18] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | [18] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| **Methanol-to-Aromatics** | capex | €/tBTX·a | 261 | 261 | 261 | 261 | [19,20] |
| | $opex_{fix}$ | % of capex p.a. | 2.5 | 2.5 | 2.5 | 2.5 | |
| | lifetime | year | 25 | 25 | 25 | 25 | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **$CO_2$ Direct Air Capture** | capex | €/tCO2·a | 730 | 338 | 237 | 199 | [21] |
| | $opex_{fix}$ | % of capex p.a. | 4 | 4 | 4 | 4 | [21] |
| | lifetime | year | 20 | 20 | 20 | 20 | [21] |
| **Heat Pump DH** | capex | $€/kW_{th}$ | 660 | 590 | 554 | 530 | [22] |
| | $opex_{fix}$ | % of capex p.a. | 0.3 | 0.3 | 0.4 | 0.4 | [22] |
| | $opex_{var}$ | $€/kWh_{th}$ | 0.002 | 0.002 | 0.002 | 0.002 | [22] |
| | lifetime | year | 25 | 25 | 25 | 25 | |
| | efficiency | - | 3.3 | 3.5 | 3.6 | 3.7 | [22] |
| **Electric Rod Heating DH** | capex | $€/kW_{th}$ | 100 | 75 | 75 | 75 | [22] |
| | $opex_{fix}$ | % of capex p.a. | 1.5 | 2 | 2 | 2 | [22] |
| | $opex_{var}$ | $€/kWh_{th}$ | 0.001 | 0.001 | 0.001 | 0.001 | [22] |
| | lifetime | year | 35 | 35 | 35 | 35 | |
| | efficiency | % | 100 | 100 | 100 | 100 | [22] |
| **Natural Gas Heating DH** | capex | $€/kW_{th}$ | 75 | 100 | 100 | 100 | [22] |
| | $opex_{fix}$ | % of capex p.a. | 3.7 | 3.7 | 3.7 | 3.7 | [22] |
| | $opex_{var}$ | $€/kWh_{th}$ | 0.0002 | 0.0002 | 0.0002 | 0.0002 | [22] |
| | lifetime | year | 35 | 35 | 35 | 35 | |
| | efficiency | % | 97 | 97 | 97 | 97 | |

**Table S17.** Direct levelised cost of electricity by major region. These costs match a defined near baseload profile.

| Region | | 2020 | 2030 | 2040 | 2050 |
|---|---|---|---|---|---|
| **Europe** | $€/MWh_{el}$ | 75.5 | 69.7 | 58.5 | 55.6 |
| **Eurasia** | $€/MWh_{el}$ | 72.7 | 56.2 | 51.5 | 57.5 |
| **MENA** | $€/MWh_{el}$ | 72.3 | 61.2 | 53.4 | 52.4 |
| **Sub-Saharan Africa** | $€/MWh_{el}$ | 62.6 | 49.2 | 42.8 | 43.8 |
| **SAARC** | $€/MWh_{el}$ | 66.4 | 67.3 | 49.6 | 45.9 |
| **Northeast Asia** | $€/MWh_{el}$ | 69.4 | 64.2 | 62.5 | 60.2 |
| **Southeast Asia** | $€/MWh_{el}$ | 62.6 | 62.2 | 49.5 | 46.2 |
| **North America** | $€/MWh_{el}$ | 70.5 | 62 | 51.9 | 53.9 |
| **South America** | $€/MWh_{el}$ | 57.7 | 48.1 | 42.3 | 37.7 |

**Table S18.** Indirect levelised cost of electricity applied to electrolysers by major region. These costs are generation costs without need for matching a load profile.

| Region | | 2020 | 2030 | 2040 | 2050 |
|---|---|---|---|---|---|
| **Europe** | $€/MWh_{el}$ | 40.3 | 28.6 | 22.7 | 17.9 |
| **Eurasia** | $€/MWh_{el}$ | 42.4 | 31.4 | 24.0 | 18.8 |
| **MENA** | $€/MWh_{el}$ | 31.7 | 24.2 | 15.7 | 11.0 |
| **Sub-Saharan Africa** | $€/MWh_{el}$ | 32.0 | 19.7 | 13.6 | 10.0 |
| **SAARC** | $€/MWh_{el}$ | 40.0 | 24.0 | 14.8 | 11.1 |
| **Northeast Asia** | $€/MWh_{el}$ | 32.1 | 26.2 | 19.1 | 13.5 |
| **Southeast Asia** | $€/MWh_{el}$ | 31.3 | 19.3 | 13.5 | 10.7 |
| **North America** | $€/MWh_{el}$ | 41.6 | 26.7 | 20.4 | 14.5 |

| | | | | | |
|---|---|---|---|---|---|
| **South America** | €/$MWh_{el}$ | 25.5 | 17.1 | 13.1 | 10.2 |

## 3. Physical Assumptions

**Table S19.** Feedstock and process energy demands for chemical technologies considered.

| Device | Demand | unit | value | Temperature level [°C] | Ref |
|---|---|---|---|---|---|
| **Water Electrolyser** | **Electricity** | $MWh_{H2,LHV}/MWh_{el}$ | 0.625-0.7 | | 3 |
| **Natural Gas-to-Ammonia** | **Feedstock** | $MWh_{th}/MWh_{NH3,LHV}$ | 1.481 | | 3 |
| | **Electricity** | $MWh_{el}/MWh_{NH3,LHV}$ | 0.016 | | 12 |
| **Coal-to-Ammonia** | **Feedstock** | $MWh_{th}/MWh_{NH3,LHV}$ | 2.011 | | 23 |
| | **Electricity** | $MWh_{el}/MWh_{NH3,LHV}$ | 0.196 | | 12 |
| **Oil-to-Ammonia** | **Feedstock** | $MWh_{th}/MWh_{NH3,LHV}$ | 2.222 | | 23 |
| | **Electricity** | $MWh_{el}/MWh_{NH3,LHV}$ | 0.196 | | |
| **Biomass-to-Ammonia** | **Feedstock** | $MWh_{th}/MWh_{NH3,LHV}$ | 2.381 | | 12 |
| | **Electricity** | $MWh_{el}/MWh_{NH3,LHV}$ | 0.265 | | 12 |
| **Natural Gas-to-Methanol** | **Feedstock** | $MWh_{th}/MWh_{MeOH,LHV}$ | 1.70 | | 12 |
| | **Electricity** | $MWh_{el}/MWh_{MeOH,LHV}$ | 0.015 | | 12 |
| **Coal-to-Methanol** | **Feedstock** | $MWh_{th}/MWh_{MeOH,LHV}$ | 2.36 | | 12 |
| | **Electricity** | $MWh_{el}/MWh_{MeOH,LHV}$ | 0.186 | | 12 |
| **Oil-to-Methanol** | **Feedstock** | $MWh_{th}/MWh_{MeOH,LHV}$ | 1.87 | | 24 |
| | **Electricity**[1] | $MWh_{el}/MWh_{MeOH,LHV}$ | 0.251 | | |
| **Biomass-to-Methanol** | **Feedstock** | $MWh_{th}/MWh_{MeOH,LHV}$ | 2.39 | | 12 |
| | **Electricity** | $MWh_{el}/MWh_{MeOH,LHV}$ | 0.251 | | 12 |
| **Power-to-Ammonia** | **Feedstock** | $MWh_{H2,LHV}/MWh_{NH3,LHV}$ | 1.148 | | 3 |
| | **Electricity** | $MWh_{el}/MWh_{NH3,LHV}$ | 0.141 | | 3 |
| **Power-to-Methanol** | **Feedstock** | $MWh_{H2,LHV}/MWh_{MeOH,LHV}$ | 1.210 | | 25 |
| | **Electricity** | $MWh_{el}/MWh_{MeOH,LHV}$ | 0.031 | | |
| | **Heat** | $MWh_{th}/MWh_{MeOH,LHV}$ | 0.396 | 100 | 25 |
| | **$CO_2$** | $t_{CO2}/MWh_{MeOH,LHV}$ | 0.264 | | |
| | **Excess heat** | $MWh_{th}/MWh_{MeOH,LHV}$ | 0.006 | 35-60 | 25–27 |
| **Naphtha Steam Cracker** | **Feedstock** | $MWh_{th}/t_{ethylene}$ | 41.2 | | 28 |
| | **Electricity** | $MWh_{el}/t_{ethylene}$ | 0.044 | | 28 |
| | **Heat** | $MWh_{th}/t_{ethylene}$ | 6.194 | 790-850 | 28,29 |
| | **Water** | $t_{H20}/t_{ethylene}$ | 400 | | 28 |
| **Ethane Steam Cracker** | **Feedstock** | $MWh_{th}/t_{ethylene}$ | 17.1 | | 28 |
| | **Electricity** | $MWh_{el}/t_{ethylene}$ | 0.140 | | 28 |
| | **Heat** | $MWh_{th}/t_{ethylene}$ | 5.833 | 790-850 | 28,29 |
| | **Water** | $t_{H20}/t_{ethylene}$ | 206 | | 28 |
| **Propane Steam Cracker** | **Feedstock** | $MWh_{th}/t_{ethylene}$ | 30.7 | | 28 |
| | **Electricity** | $MWh_{el}/t_{ethylene}$ | 0.180 | | 28 |
| | **Heat** | $MWh_{th}/t_{ethylene}$ | 6.833 | | 28 |
| | **Water** | $t_{H20}/t_{ethylene}$ | 206 | | 28 |
| **Butane Steam Cracker** | **Feedstock** | $MWh_{th}/t_{ethylene}$ | 31.6 | | 28 |
| | **Electricity** | $MWh_{el}/t_{ethylene}$ | 0.180 | | 28 |
| | **Heat** | $MWh_{th}/t_{ethylene}$ | 6.899 | 790-850 | 28,29 |
| | **Water** | $t_{H20}/t_{ethylene}$ | 206 | | 28 |
| **Gas Oil Steam Cracker** | **Feedstock** | $MWh_{th}/t_{ethylene}$ | 43.3 | | 30 |
| | **Electricity** | $MWh_{el}/t_{ethylene}$ | 0.3 | | 28 |
| | **Heat** | $MWh_{th}/t_{ethylene}$ | 8.694 | 790-850 | 28,29 |
| | **Water** | $t_{H20}/t_{ethylene}$ | 206 | | 28 |
| **Propane Dehydrogenation** | **Feedstock** | $MWh_{th}/t_{propylene}$ | 16.7 | | 29 |

| | | | | | |
|---|---|---|---|---|---|
| | **Electricity** | $MWh_{el}/t_{propylene}$ | 0.078 | | [29] |
| | **Heat** | $MWh_{th}/t_{propylene}$ | 2.632 | 500-680 | [29] |
| | **Water** | $t_{H20}/t_{propylene}$ | 95.4 | | [29] |
| **Refinery Oil Catalytic Cracking** | **Feedstock** | $MWh_{th}/t_{propylene}$ | 58.6 | | [29] |
| | **Electricity** | $MWh_{el}/t_{propylene}$ | 0.176 | | [29] |
| | **Heat** | $MWh_{th}/t_{propylene}$ | 1.805 | 530-560 | [29] |
| | **Water** | $t_{H20}/t_{propylene}$ | 336 | | [29] |
| **Naphtha Catalytic Reforming** | **Feedstock** | $MWh_{th}/t_{BTX}$ | 24.80 | | [17] |
| | **Electricity** | $MWh_{el}/t_{BTX}$ | 0.188 | | [17] |
| | **Heat** | $MWh_{th}/t_{BTX}$ | 1.947 | 525 | [17] |
| **Methanol-to-Olefins** | **Feedstock** | $MWh_{th}/t_{olefin}$ | 16.338 | | [20] |
| | **Electricity** | $MWh_{el}/t_{olefin}$ | 2.150 | | [20] |
| | **Heat** | $MWh_{th}/t_{olefin}$ | 0.313 | 500 | [20,29] |
| | **Excess Heat** | $MWh_{th}/t_{olefin}$ | 1.239 | 500 | [31,32] |
| | **Water byproduct** | $t_{H2O}/t_{olefin}$ | 1.685 | | [31] |
| **Methanol-to-Aromatics** | **Feedstock** | $MWh_{th}/t_{BTX}$ | 34.47 | | [19,20] |
| | **Electricity** | $MWh_{el}/t_{BTX}$ | 0.702 | | [19,20] |
| | **Heat** | $MWh_{th}/t_{BTX}$ | 1.577 | 400 | [19,20] |
| | **Excess Heat** | $MWh_{th}/t_{BTX}$ | 2.838 | 400 | [31,33] |
| | **Water byproduct** | $t_{H2O}/t_{BTX}$ | 3.224 | | [19,34] |

[1] Electricity demand for Biomass-to-Methanol route assumed

[2] HVC refers to ethylene, propylene, benzene, toluene, and mixed xylenes

# 4. Supplementary Results

## 4.1. Global Chemical and Feedstock Results

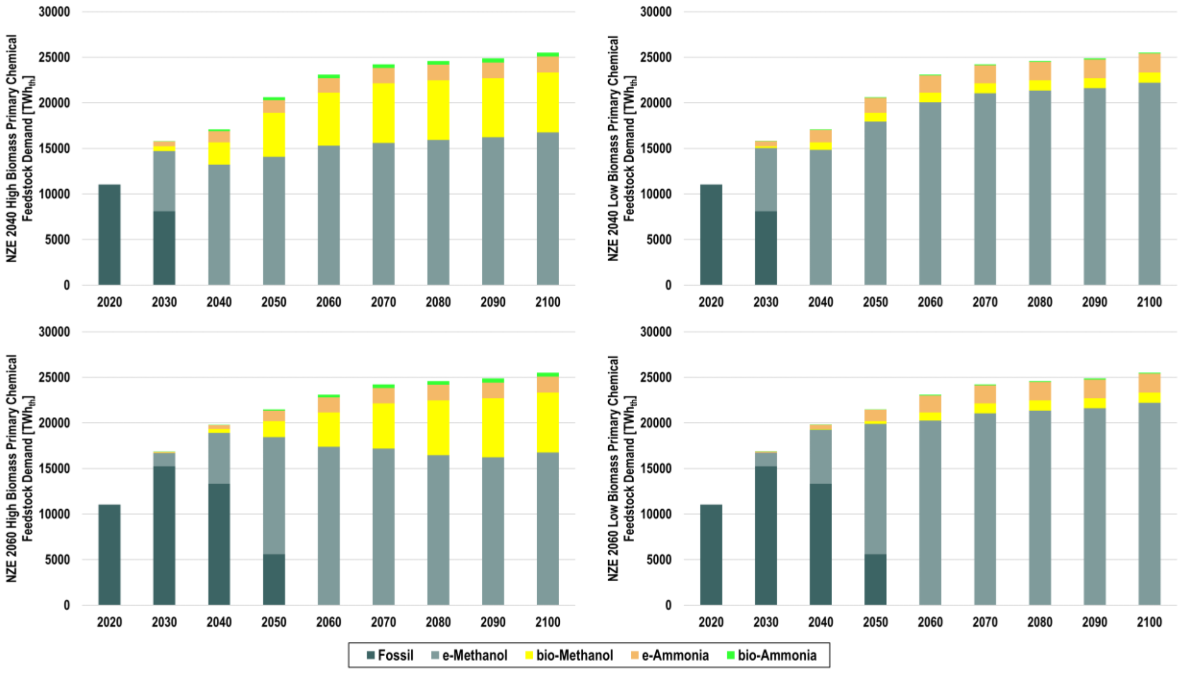


**Figure S1.** Chemical feedstock demands for the global chemical industry from 2020 to 2100 in 10-year intervals for the NZE 2040H (top left), NZE 2040L (top right), NZE 2060H (bottom left), and NZE2060L scenarios. Fossil feedstocks compose coal, fossil methane, and all oil feedstocks for HVC production.

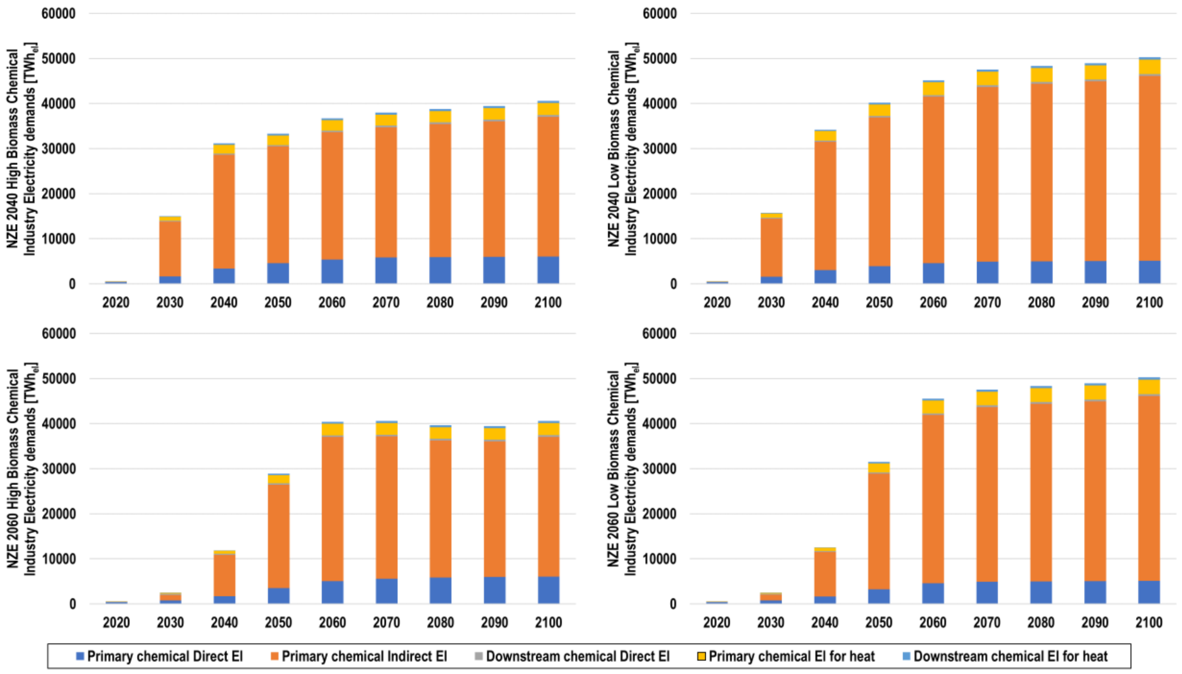


**Figure S2.** Direct (for chemical production plants), indirect (for water electrolysis), and heating electricity demands for the NZE 2040H (top left), NZE 2040L (top right), NZE 2060H (bottom left), and NZE 2060L (bottom right) scenarios.

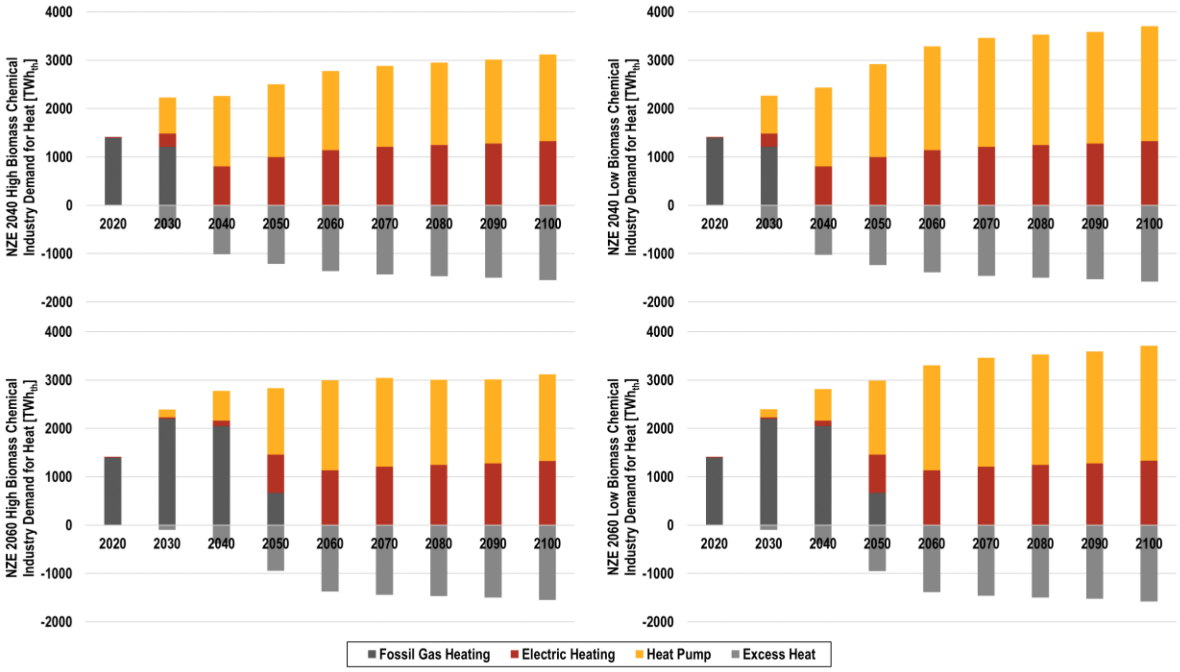


**Figure S3.** Process heating demands and excess heat from exothermic reactions in the Power-to-Methanol, MTO, and MTA processes from 2020 to 2100 for NZE2040H (top left), NZE 2040L (top right), NZE 2060H (bottom left), and NZE 2060L (bottom right) scenarios. Note that the value listed for heat pumps is the electricity input and is thus in TWh$_{el}$.

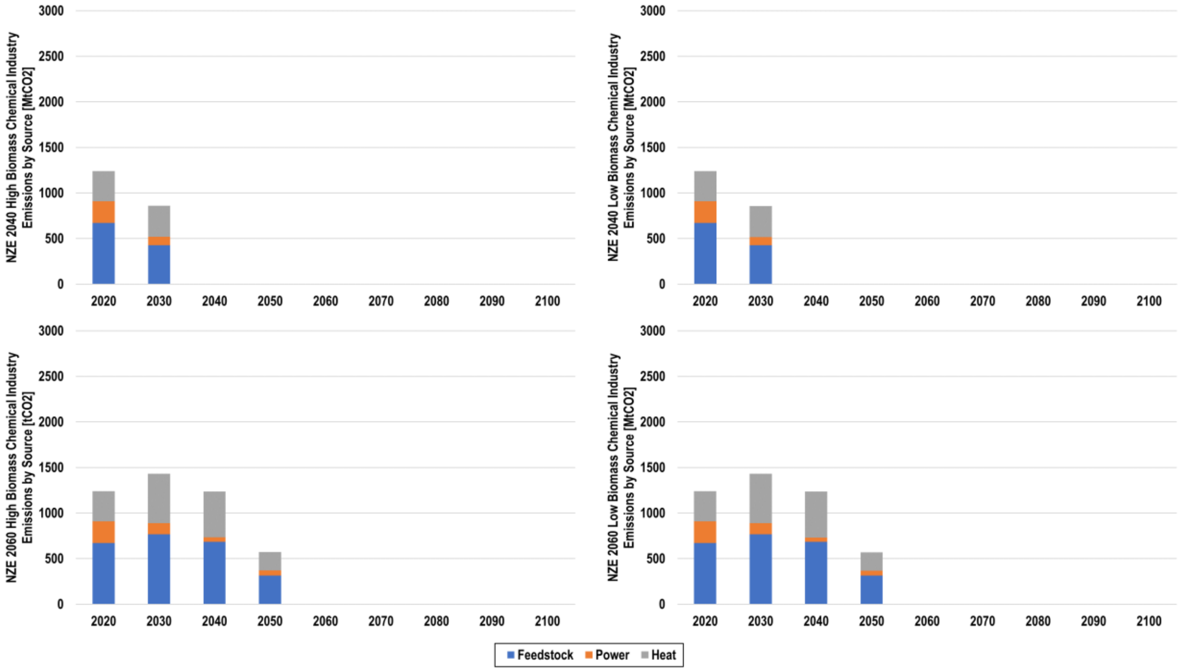


**Figure S4.** Chemical industry emissions by source for the NZE 2040H (top left), NZE 2040L (top right), NZE 2060H (bottom left), and NZE 2060L (bottom right) scenarios.

## 4.2. Global Chemical Flows

### 4.2.1. BAU

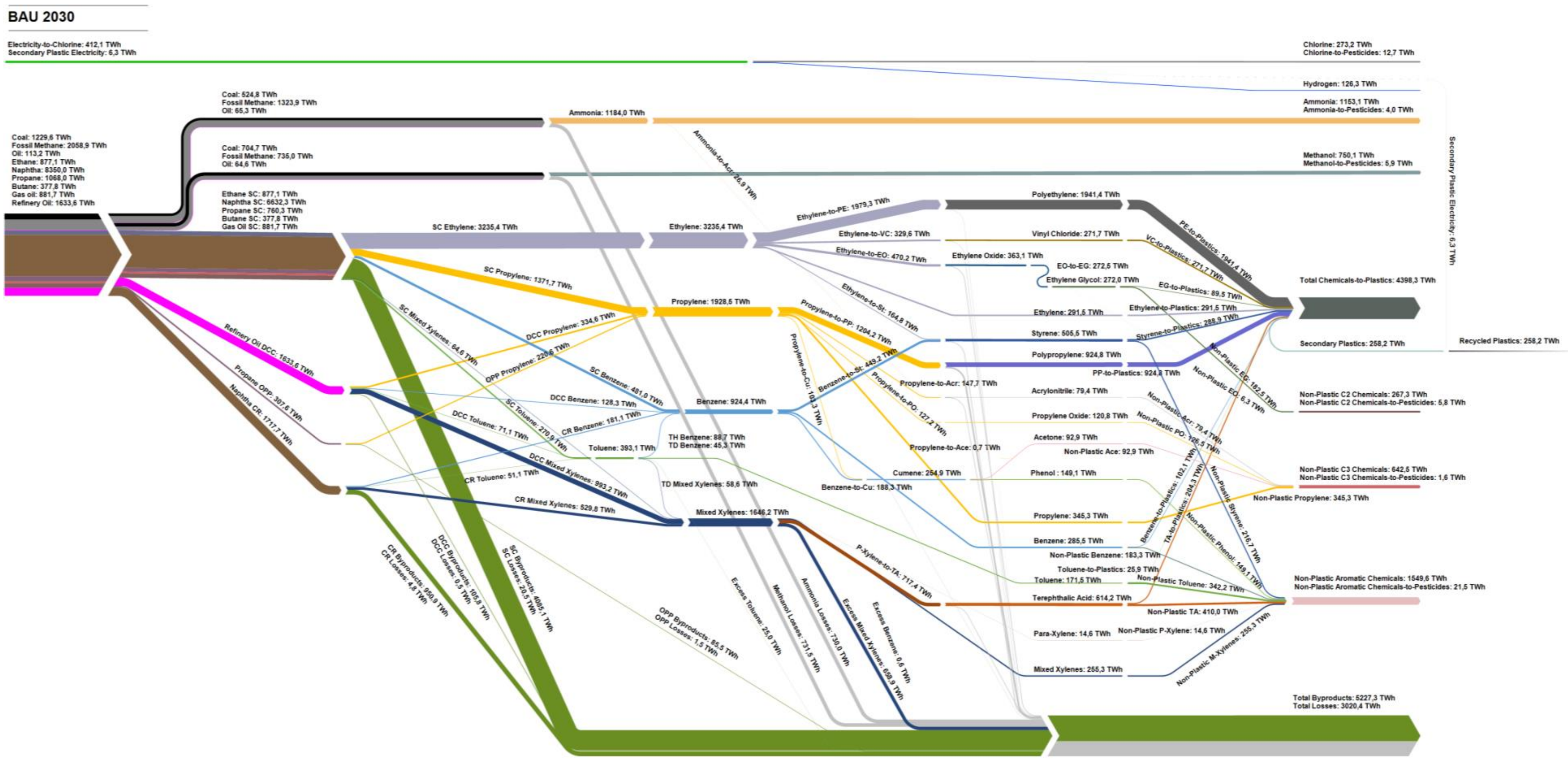


**Figure S5.** Global chemical flows in 2030 for the BAU scenario.

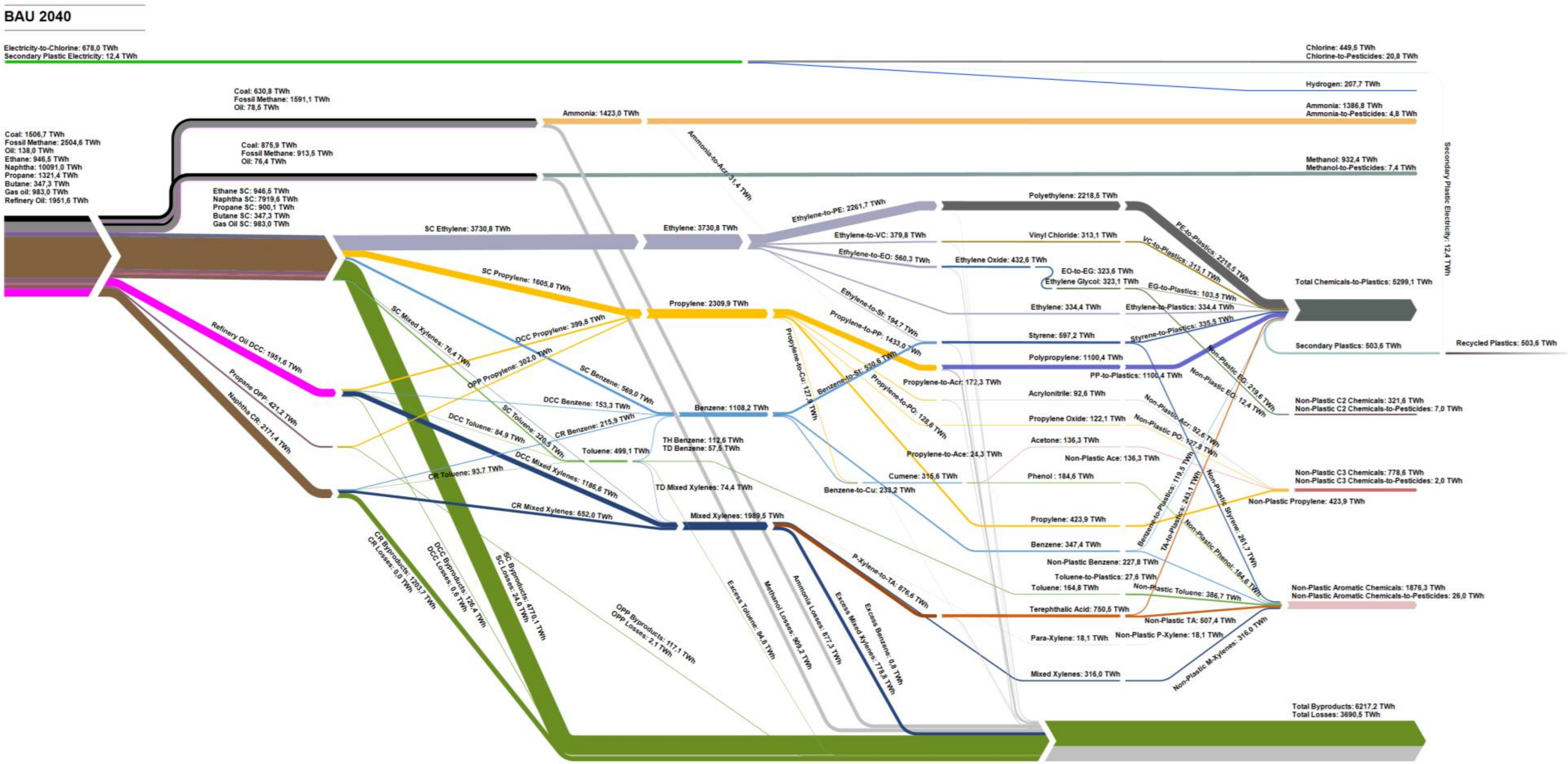


**Figure S6.** Global chemical flows in 2040 for the BAU scenario.

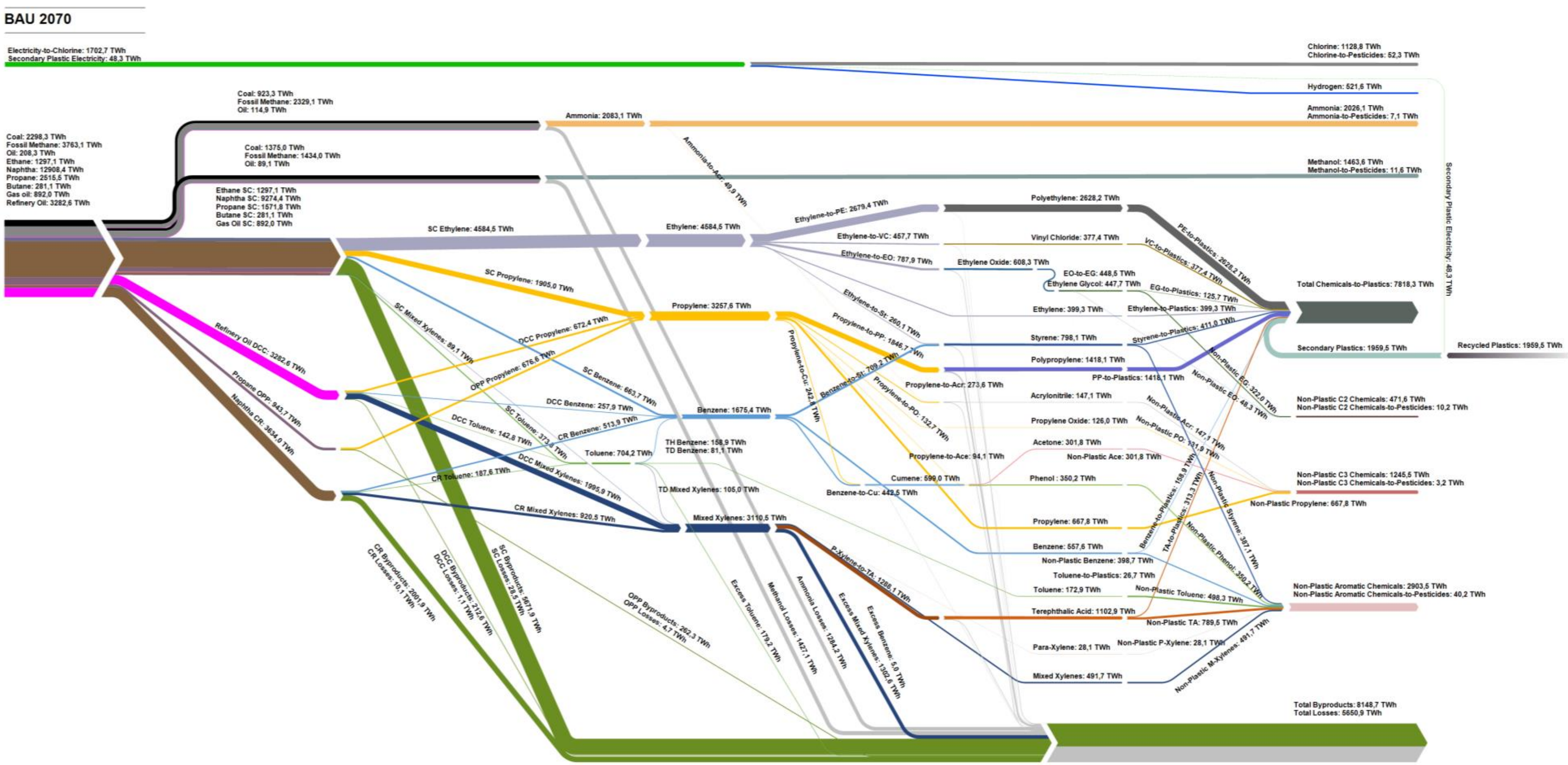


**Figure S7**. Global chemical flows in 2070 for the BAU scenario.

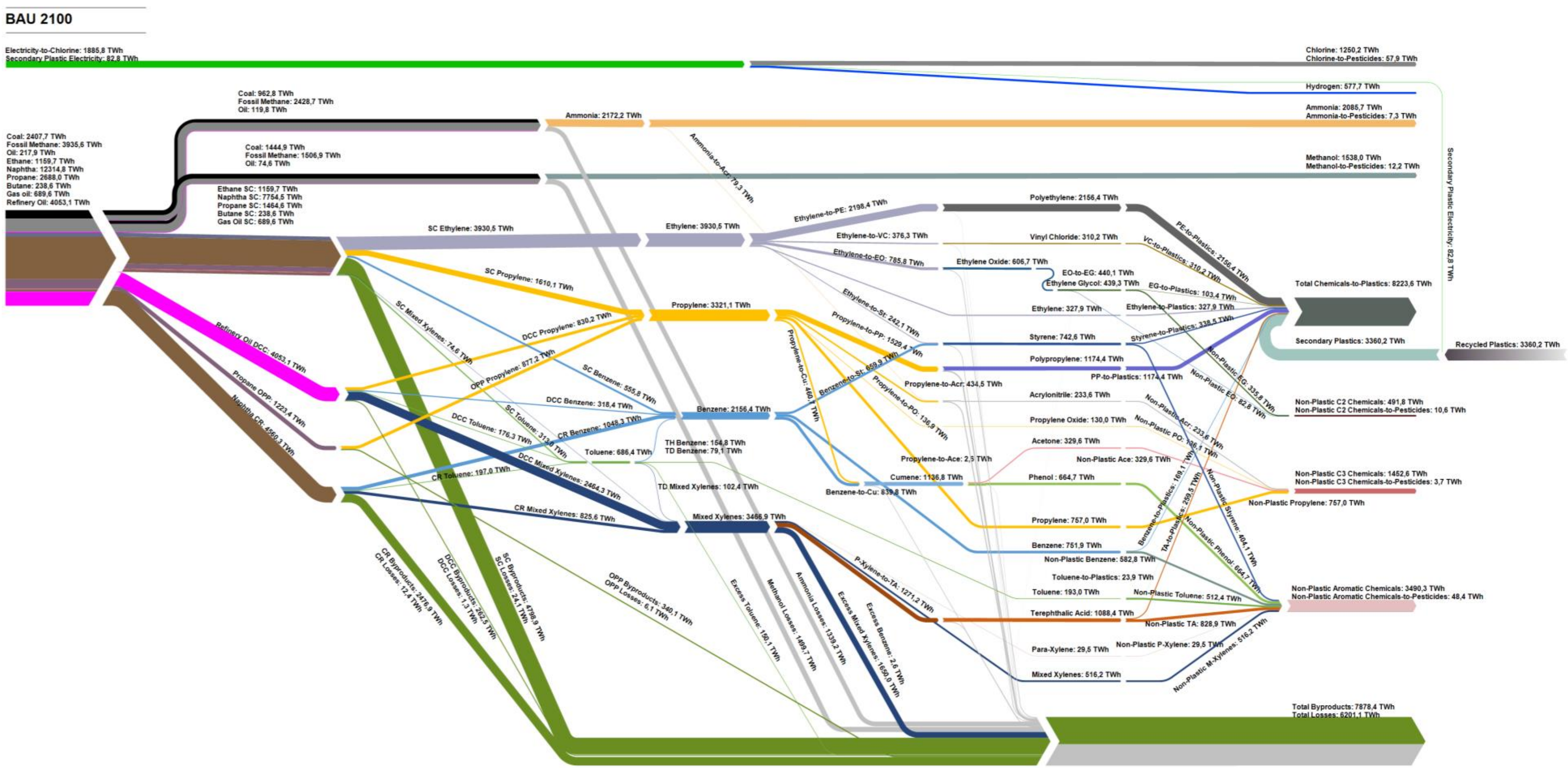

**Figure S8**. Global chemical flows in 2100 for the BAU scenario.

### 4.2.2. NZE 2050H

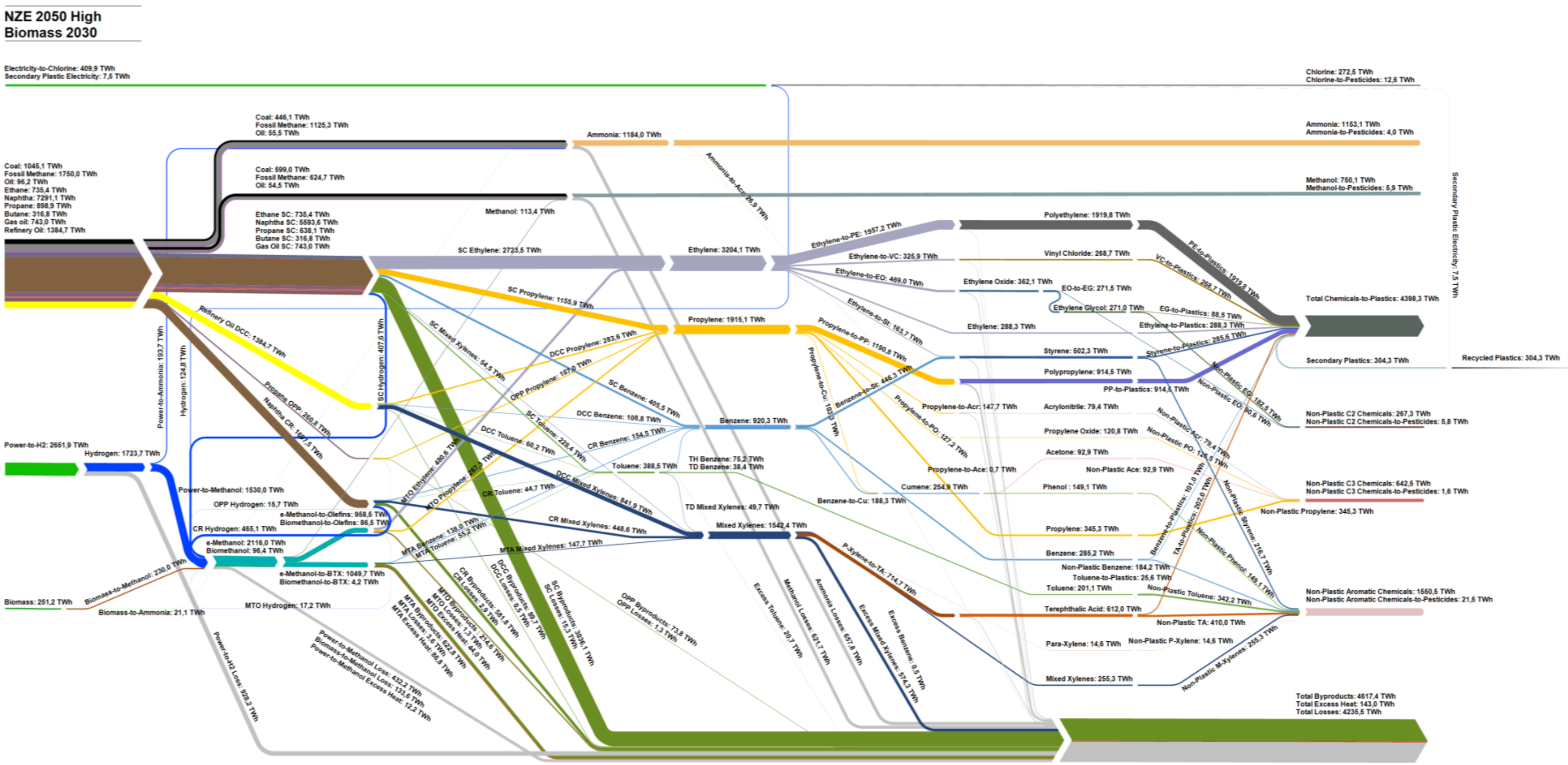


**Figure S9**. Global chemical flows in 2030 for the NZE2050H scenario.

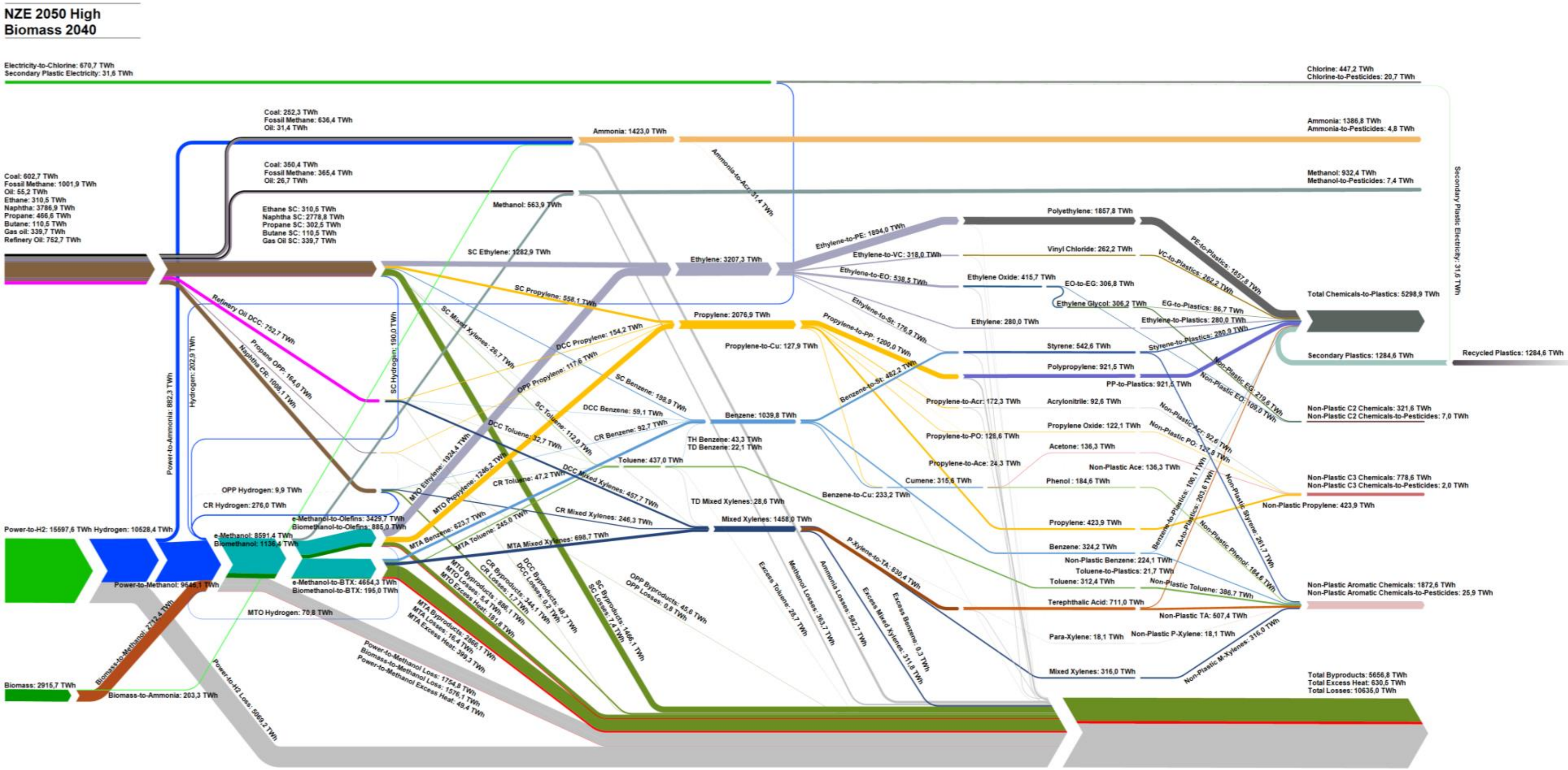


**Figure S10**. Global chemical flows in 2040 for the NZE2050H scenario.

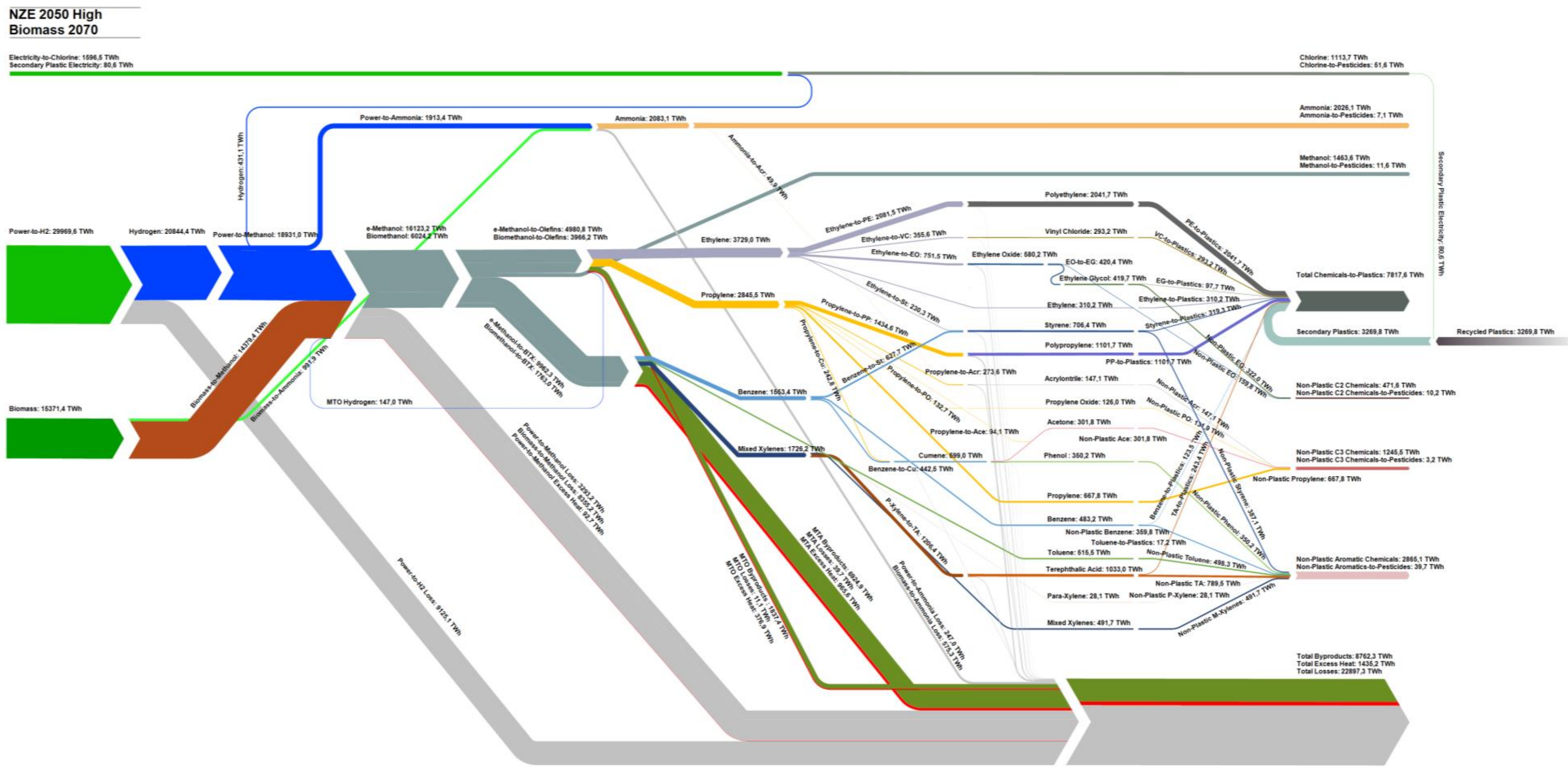


**Figure S11**. Global chemical flows in 2070 for the NZE2050H scenario.

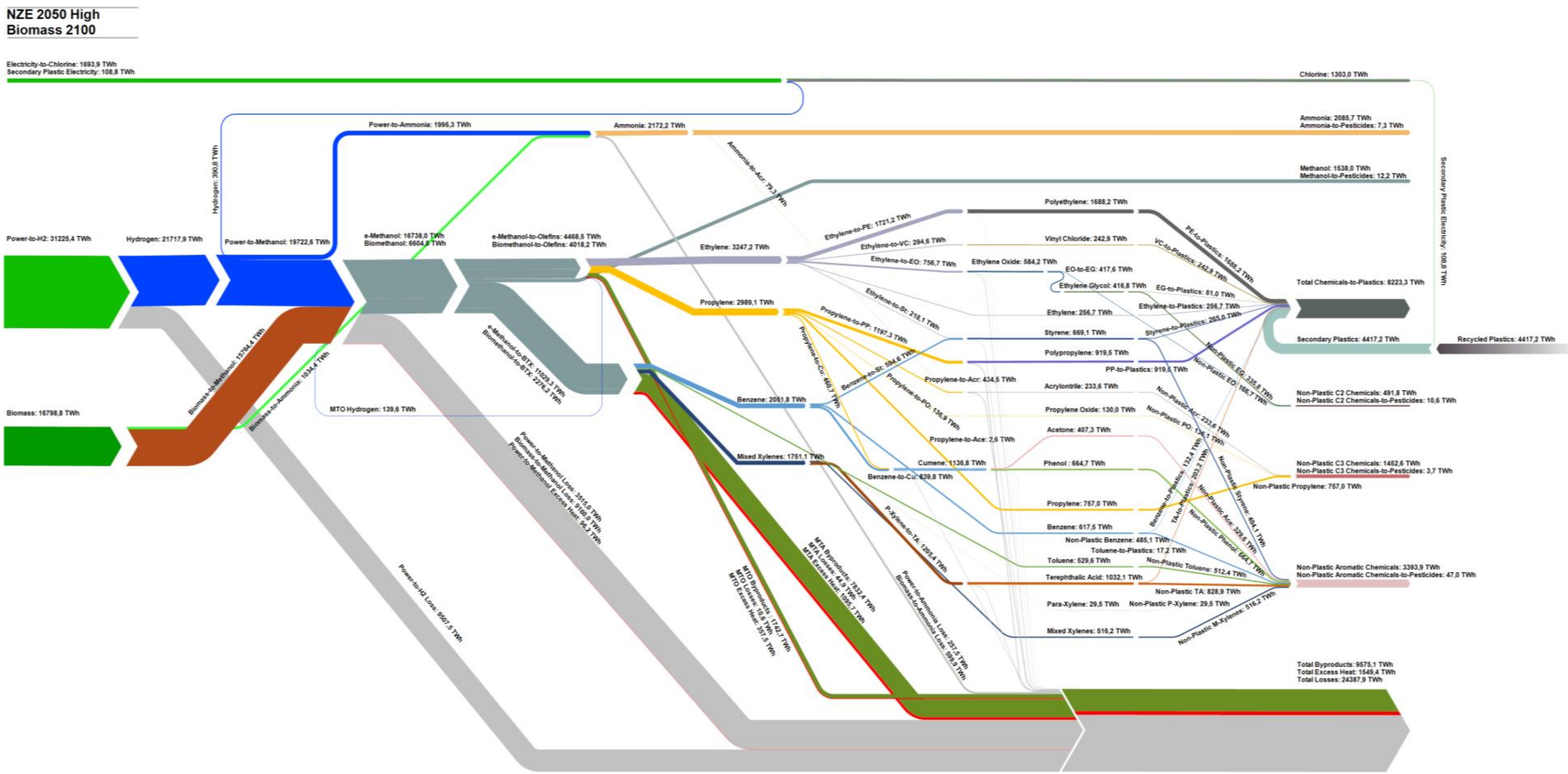


**Figure S12**. Global chemical flows in 2100 for the NZE2050H scenario.

### 4.2.3. NZE 2050L

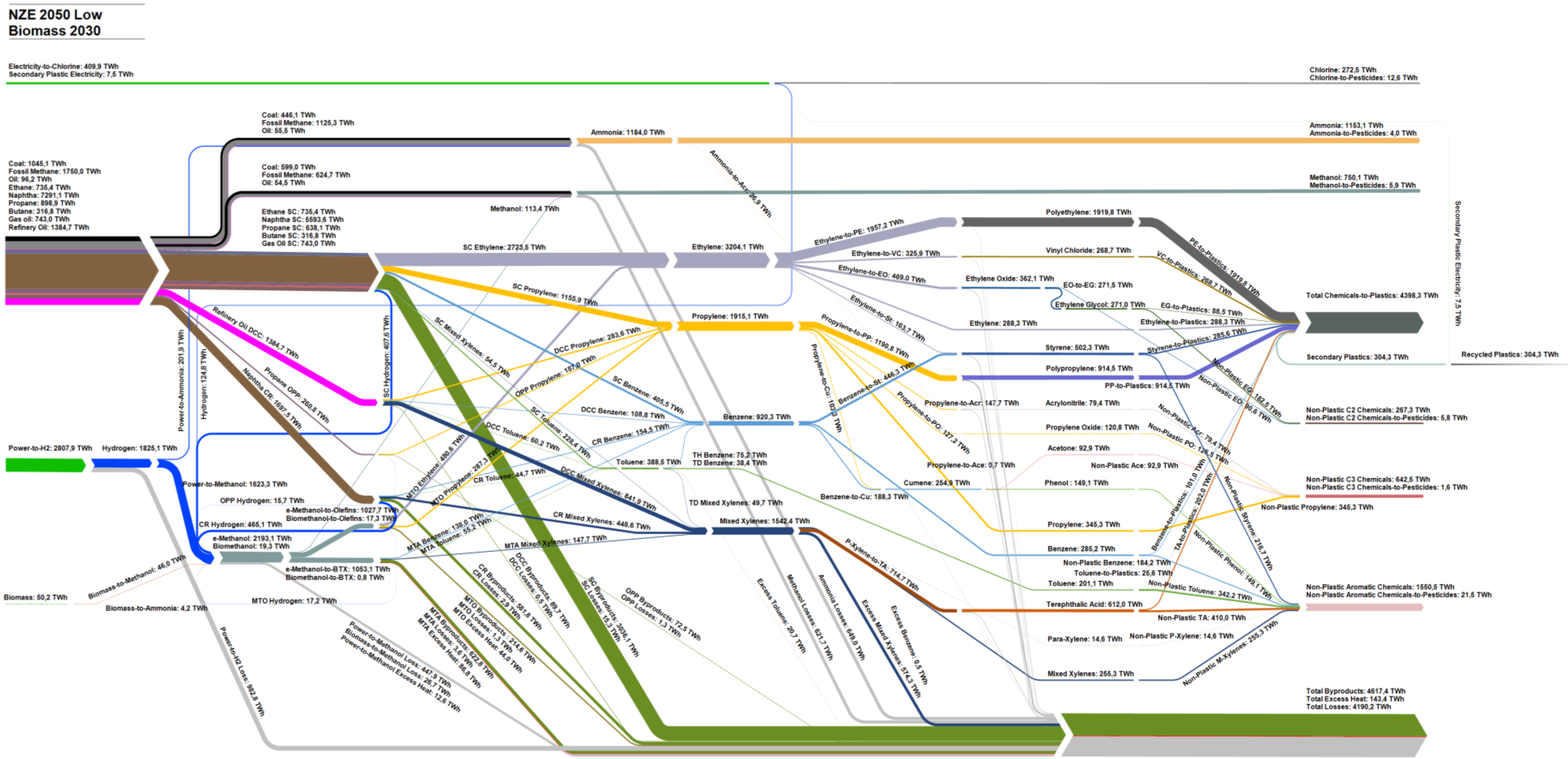


**Figure S13**. Global chemical flows in 2030 for the NZE2050L scenario.

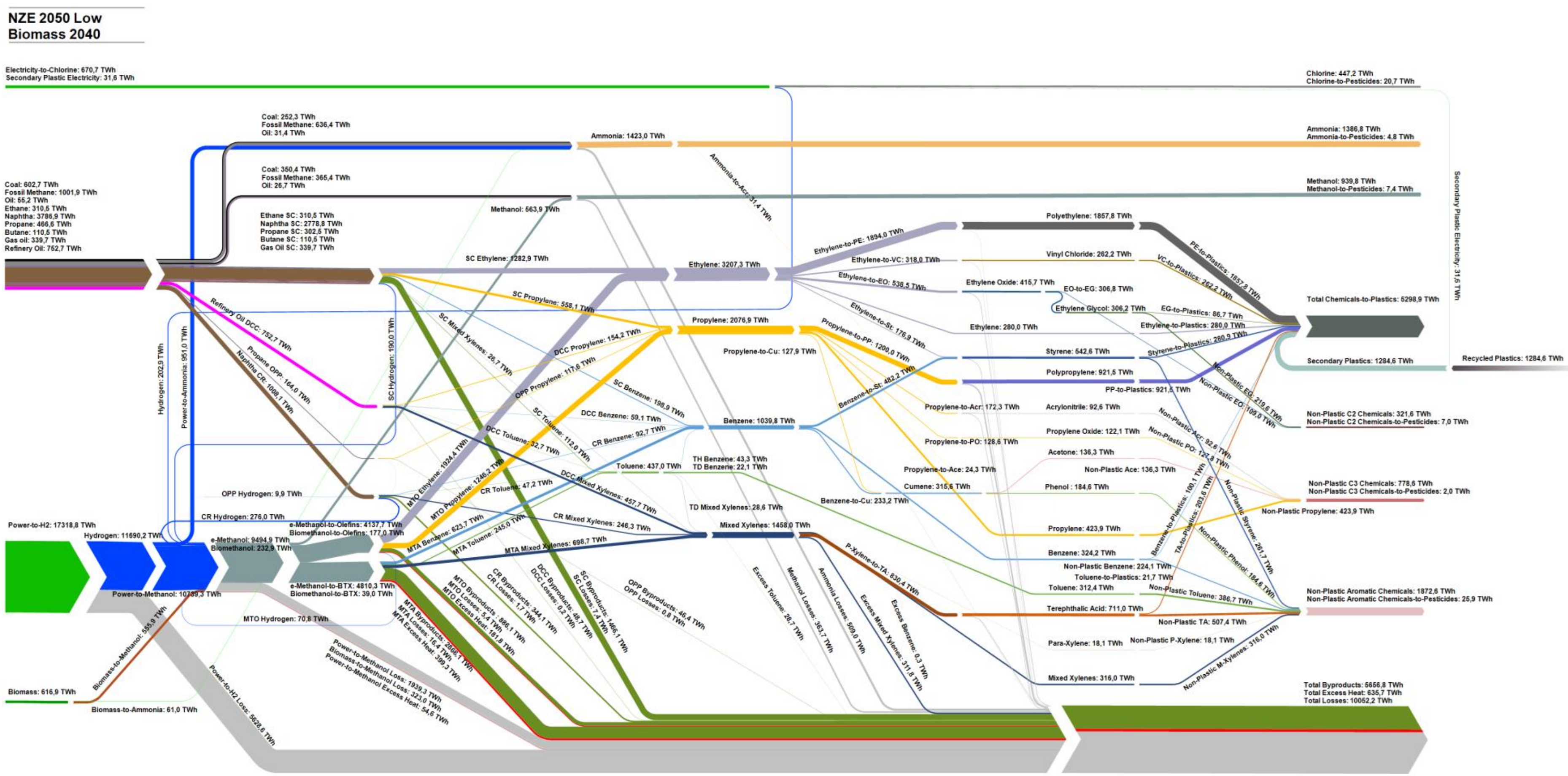

**Figure S14**. Global chemical flows in 2040 for the NZE2050L scenario.

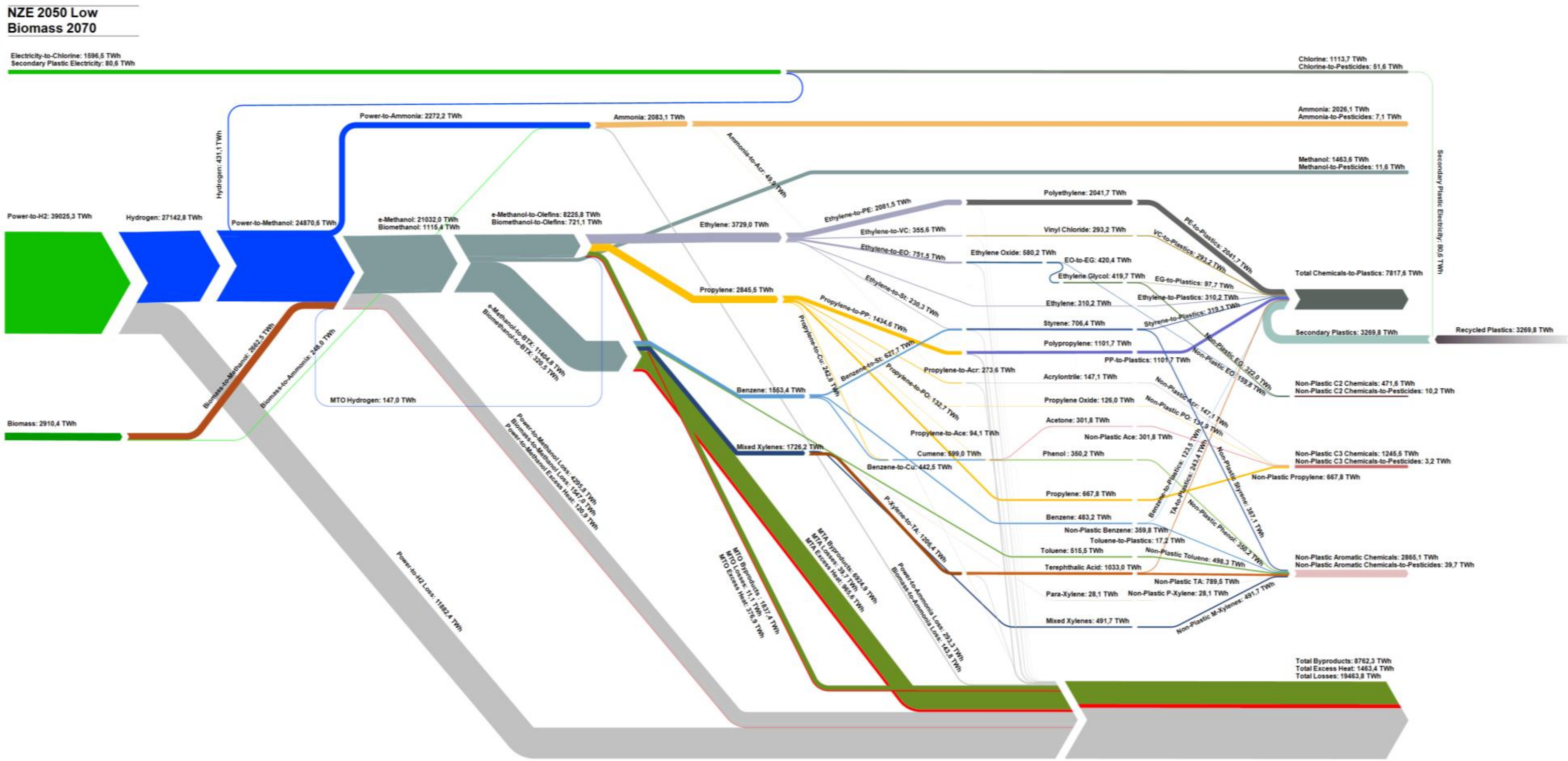

**Figure S15**. Global chemical flows in 2070 for the NZE2050L scenario.

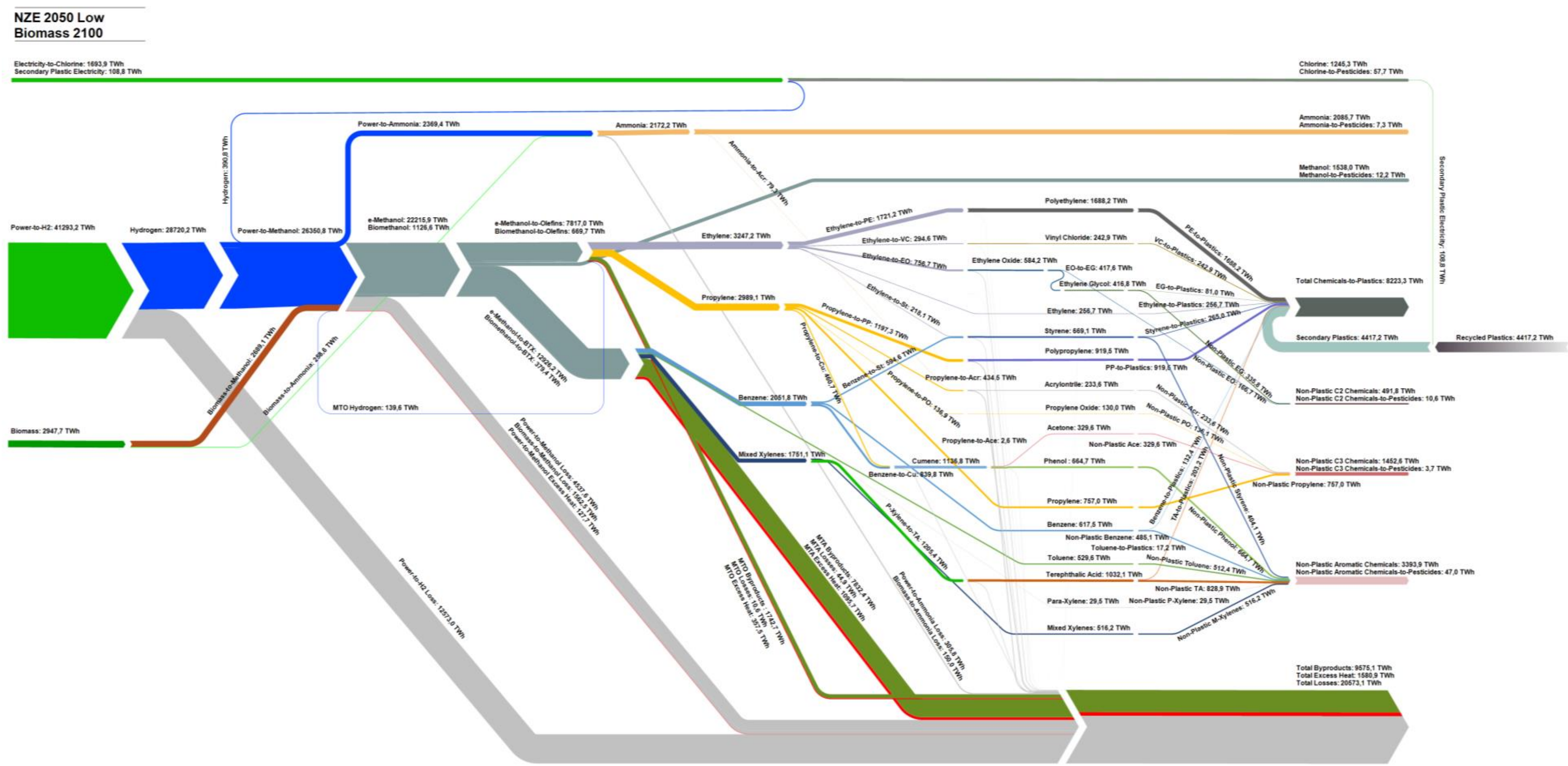


**Figure S16**. Global chemical flows in 2100 for the NZE2050L scenario.

## 4.3. Geographical Results

### 4.3.1. BAU

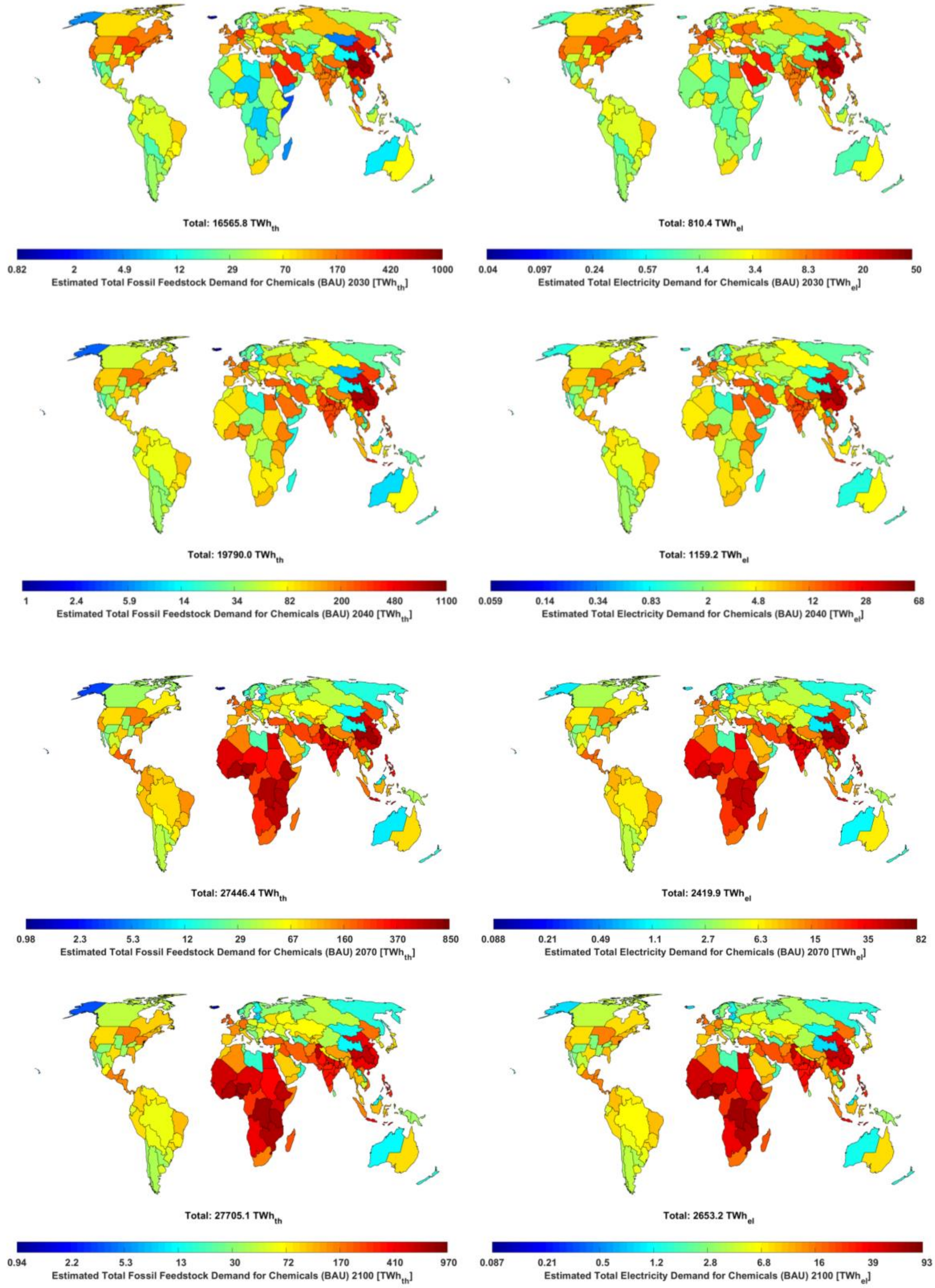


**Figure S17.** Total fossil feedstock (left) and electricity demand (right) in 2030 (top), 2040 (second from top), 2070 (second from bottom), and 2100 (bottom) for the BAU scenario.

### 4.3.2. NZE 2050

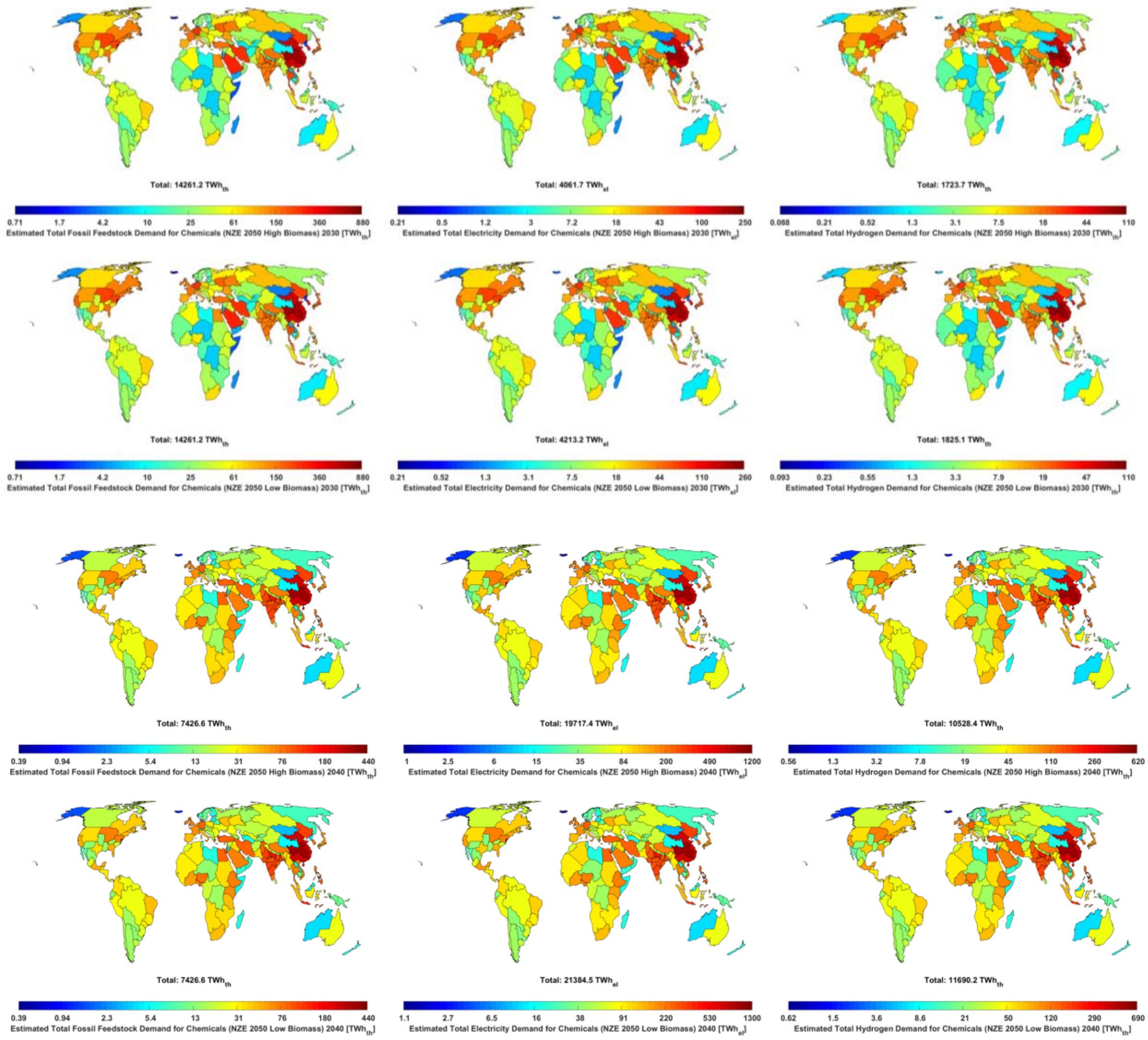


**Figure S18.** Total fossil feedstock (left), electricity (middle), and e-hydrogen demands (right) in 2030 (top) and 2040 (bottom) for the NZE 2050H (top of each row) and NZE 2050L (bottom of each row).

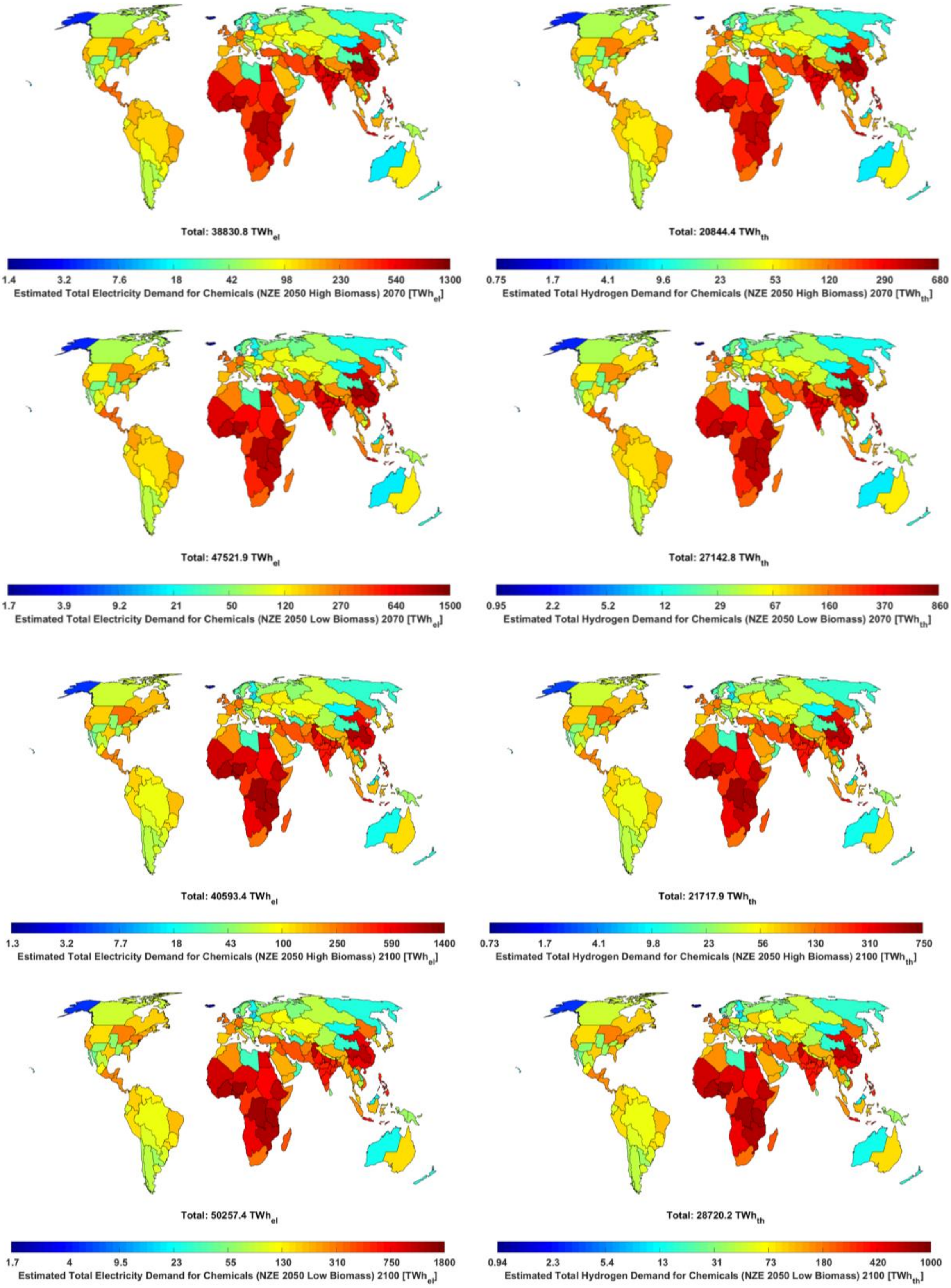


**Figure S19.** Total electricity (left) and e-hydrogen demands (right) in 2070 (top) and 2100 (bottom) for the NZE 2050H (top of each row) and NZE 2050L (bottom of each row).

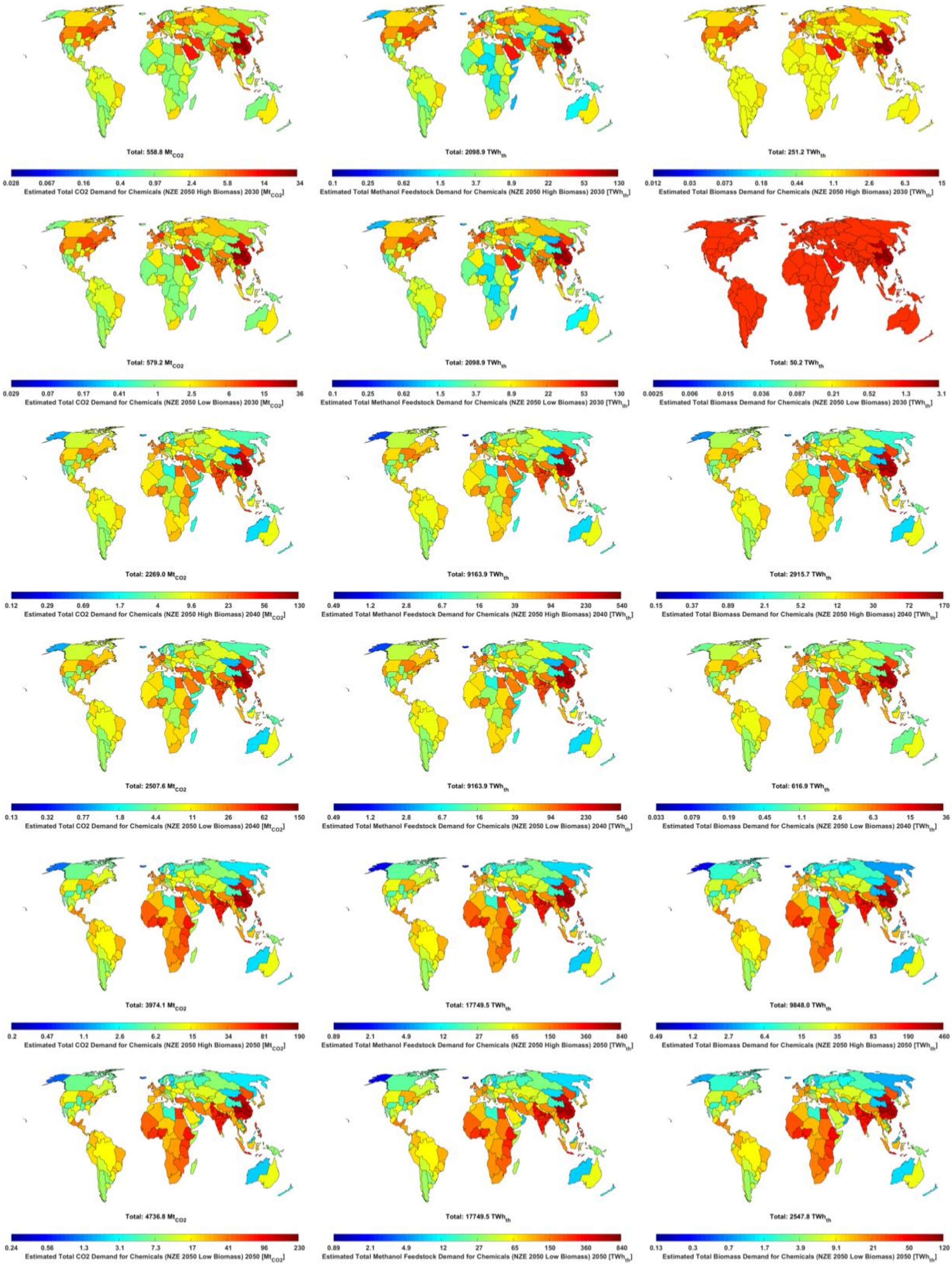


**Figure S20.** Total $CO_2$ (left), methanol feedstock (middle), and biomass demands (right) in 2030 (top), 2040 (middle), and 2050 (bottom) for the NZE 2050H (top of each row) and NZE 2050L (bottom of each row).

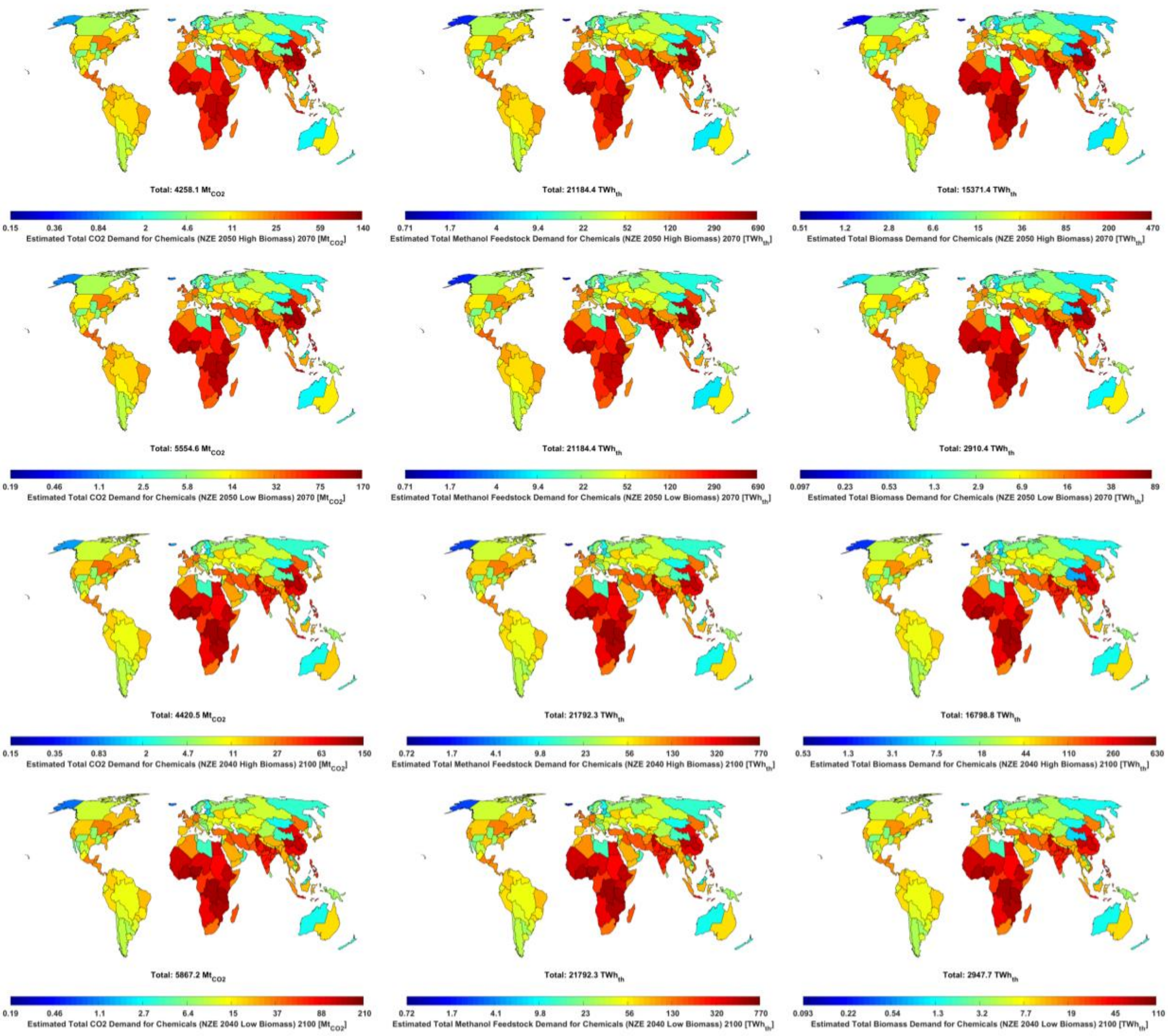


**Figure S21.** Total $CO_2$ (left), methanol feedstock (middle), and biomass demands (right) in 2070 (top), and 2100 (bottom) for the NZE 2050H (top of each row) and NZE 2050L (bottom of each row).

### 4.3.3. NZE 2040

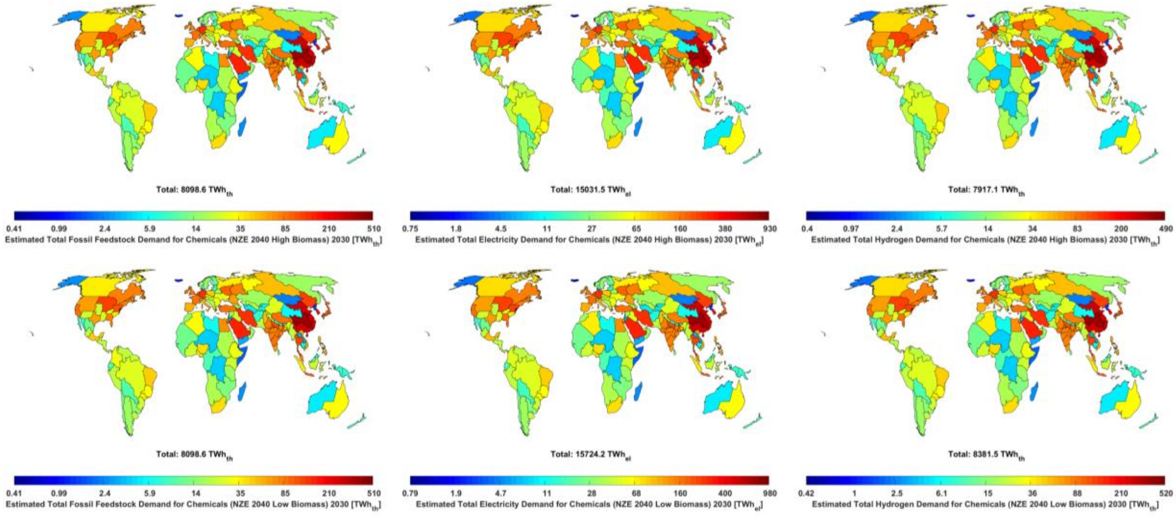


**Figure S22.** Total fossil feedstock (left), electricity (middle), and e-hydrogen demands (right) in 2030 for the NZE 2040H (top) and NZE 2040L (bottom).

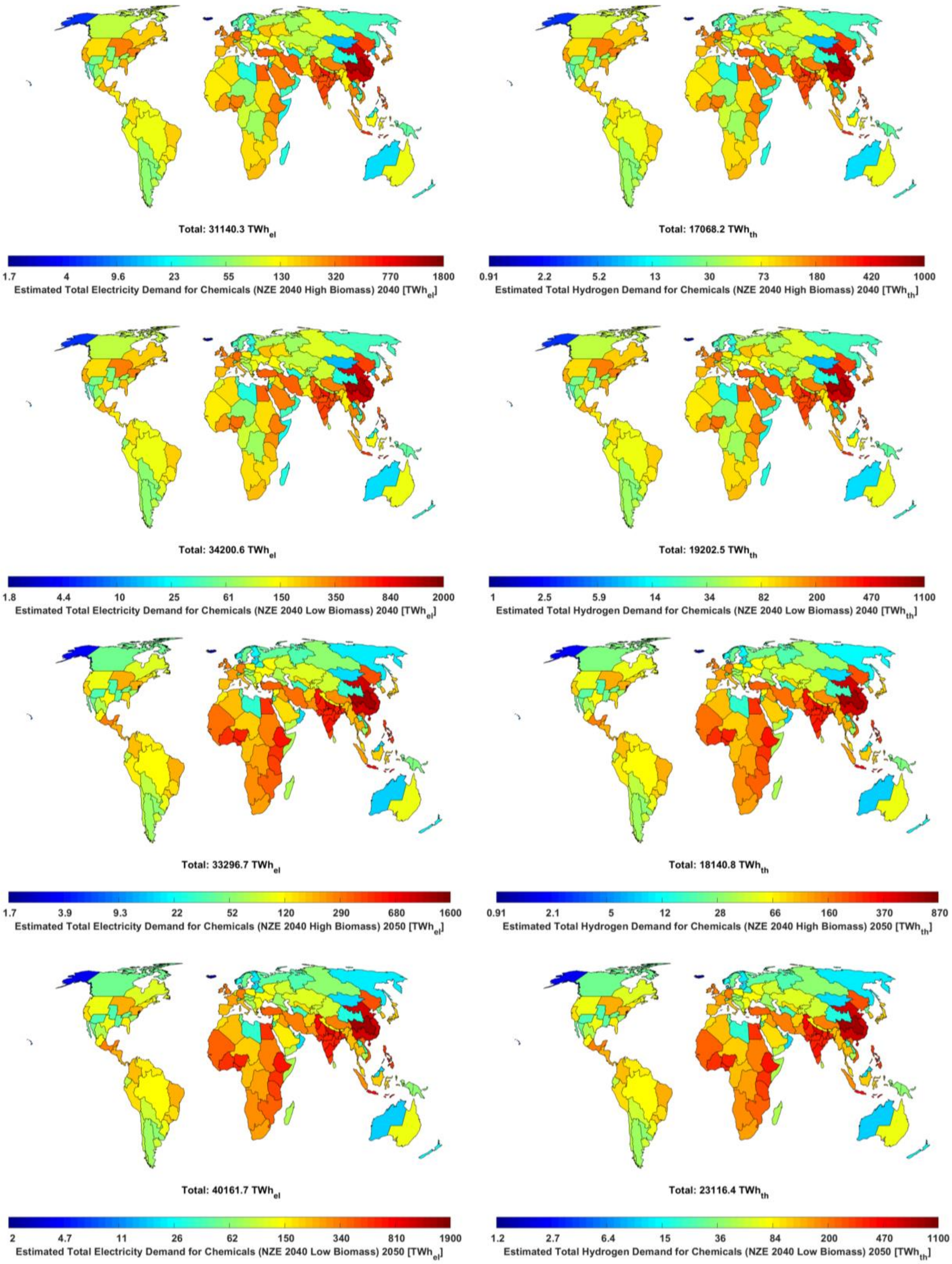


**Figure S23.** Total electricity (left) and e-hydrogen demands (right) in 2040 (top) and 2050 (bottom) for the NZE 2040H (top of each row) and NZE 2040L (bottom of each row).

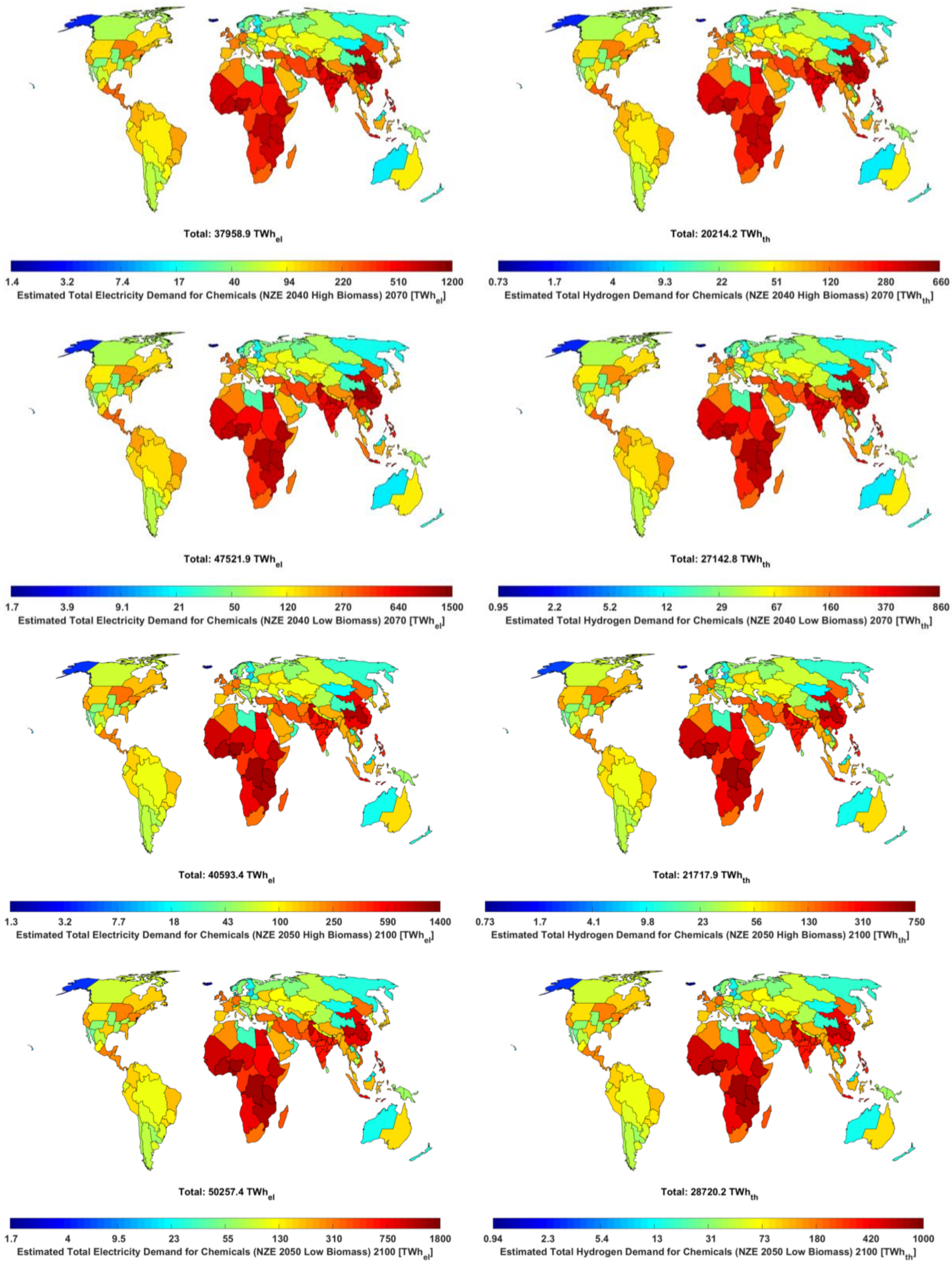


**Figure S24.** Total electricity (left) and e-hydrogen demands (right) in 2070 (top) and 2100 (bottom) for the NZE 2040H (top of each row) and NZE 2040L (bottom of each row).

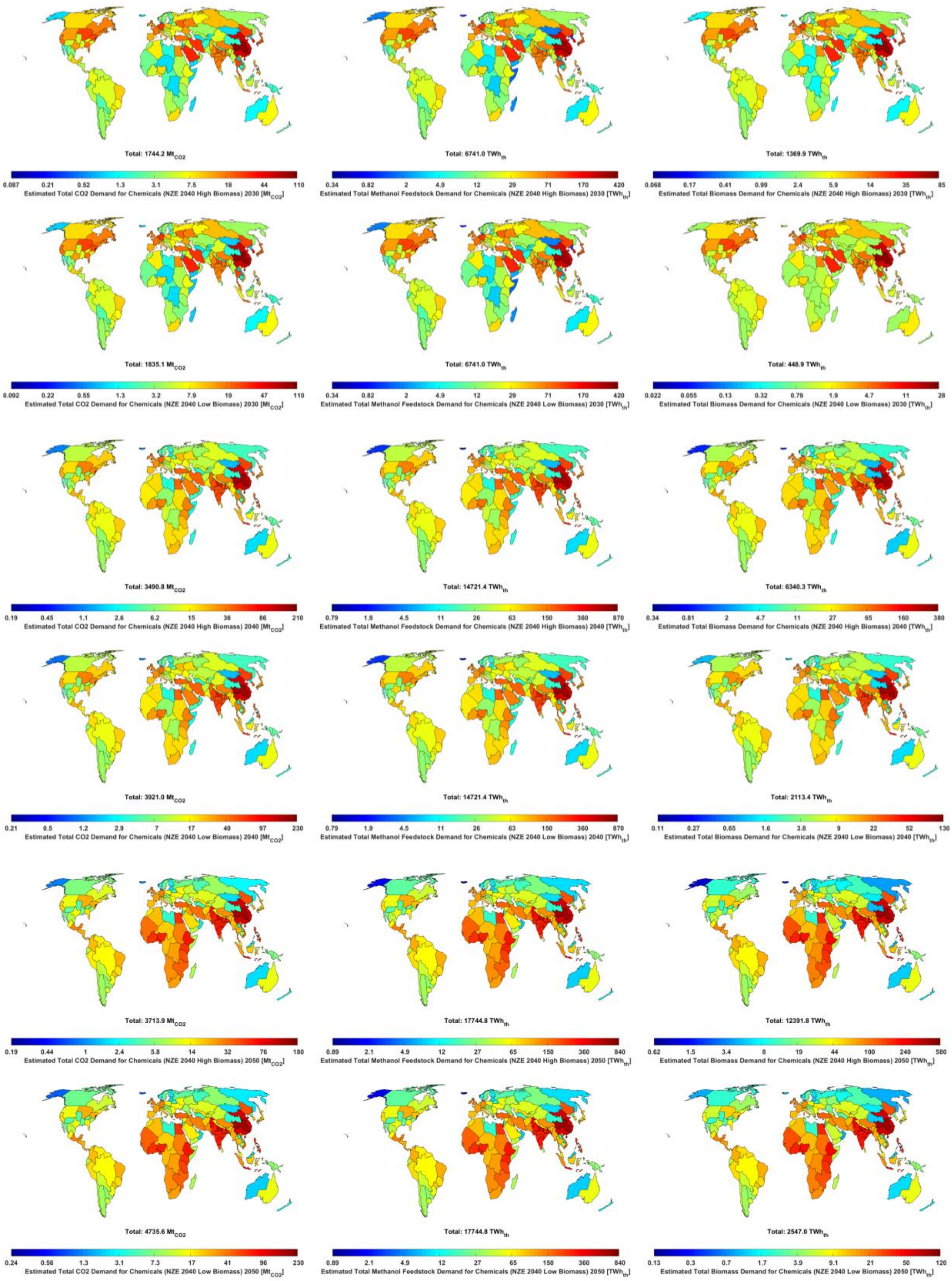


**Figure S25.** Total $CO_2$ (left), methanol feedstock (middle), and biomass demands (right) in 2030 (top), 2040 (middle), and 2050 (bottom) for the NZE 2040H (top of each row) and NZE 2040L (bottom of each row).

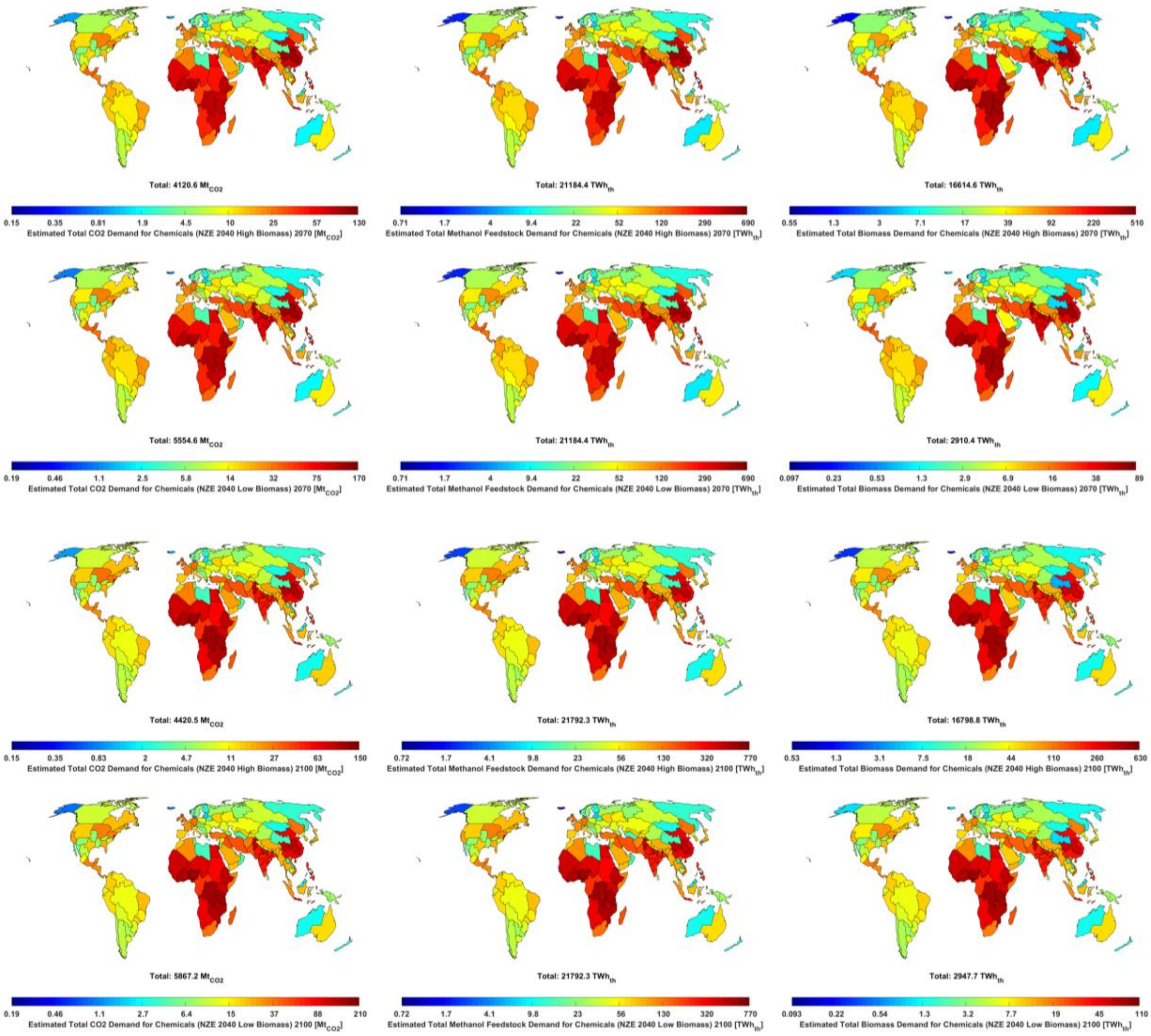


**Figure S26.** Total $CO_2$ (left), methanol feedstock (middle), and biomass demands (right) in 2070 (top), and 2100 (bottom) for the NZE 2040H (top of each row) and NZE 2040L (bottom of each row).

### 4.3.4. NZE 2060

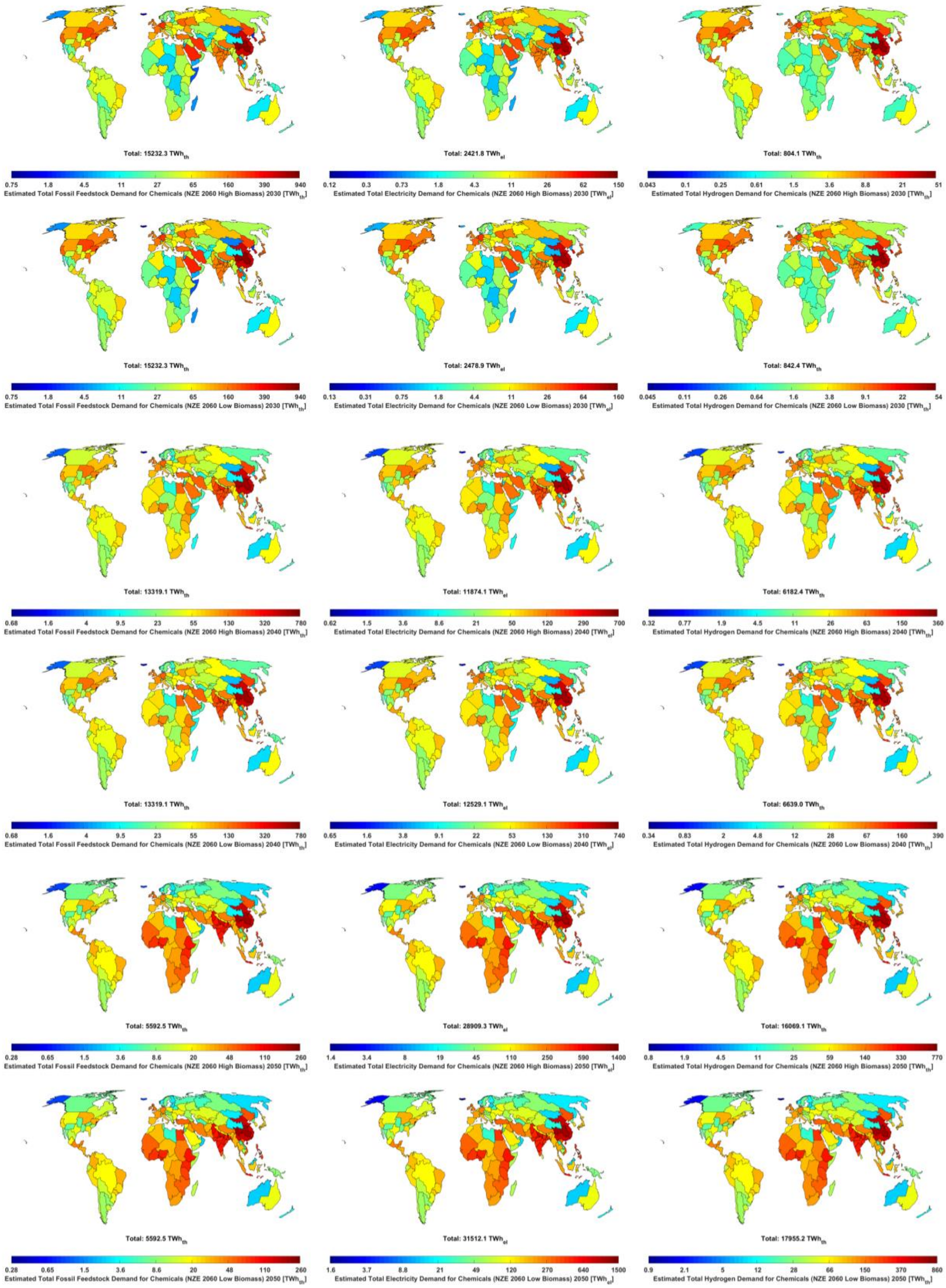


**Figure S27.** Total fossil feedstock (left), electricity (middle), and e-hydrogen demands (right) in 2030 (top), 2040 (middle), and 2050 (bottom) for the NZE 2060H (top) and NZE 2060L (bottom).

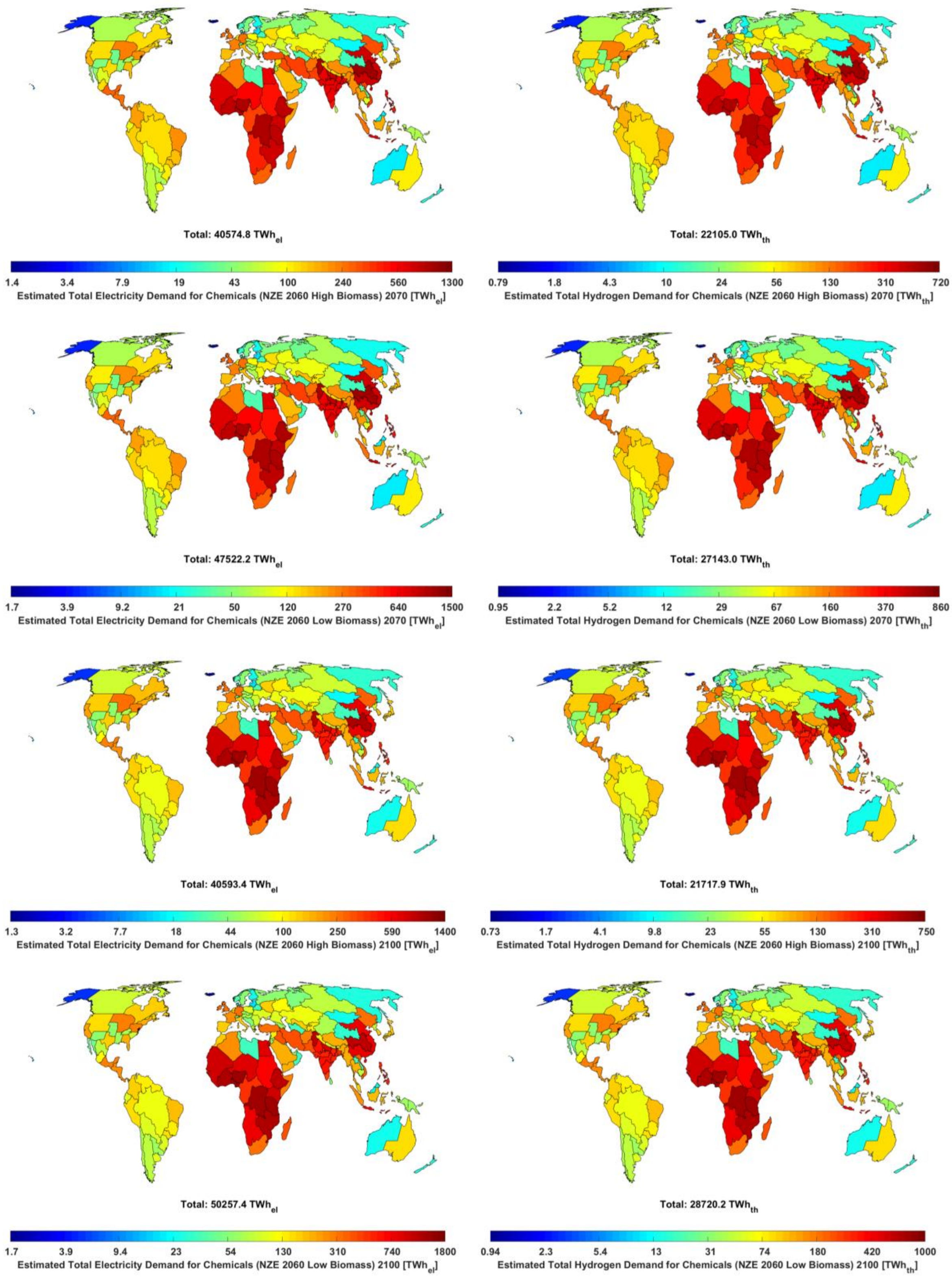


**Figure S28.** Total electricity (left) and e-hydrogen demands (right) in 2070 (top) and 2100 (bottom) for the NZE 2040H (top of each row) and NZE 2040L (bottom of each row).

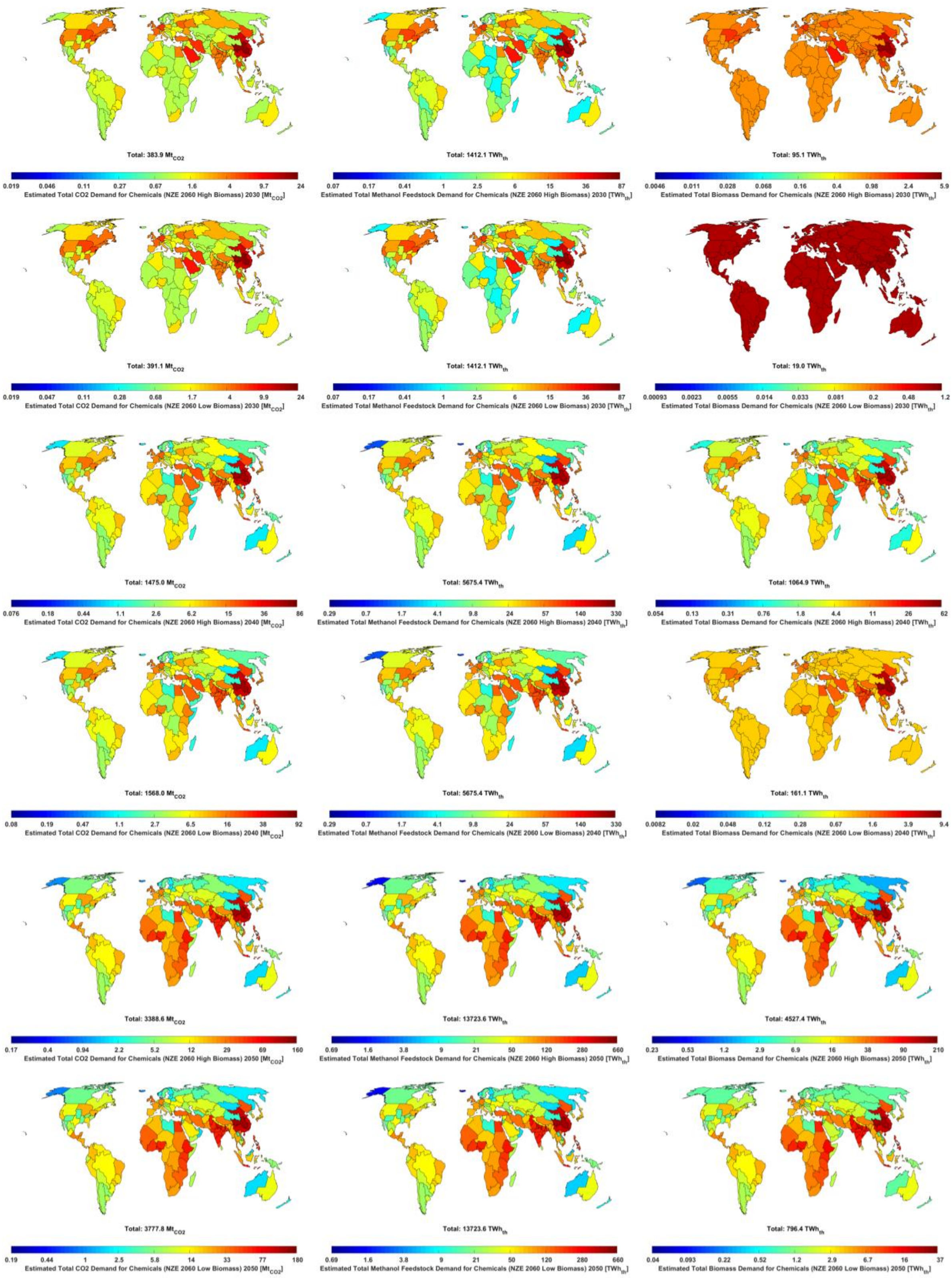


**Figure S29.** Total $CO_2$ (left), methanol feedstock (middle), and biomass demands (right) in 2030 (top), 2040 (middle), and 2050 (bottom) for the NZE 2060H (top of each row) and NZE 2060L (bottom of each row).

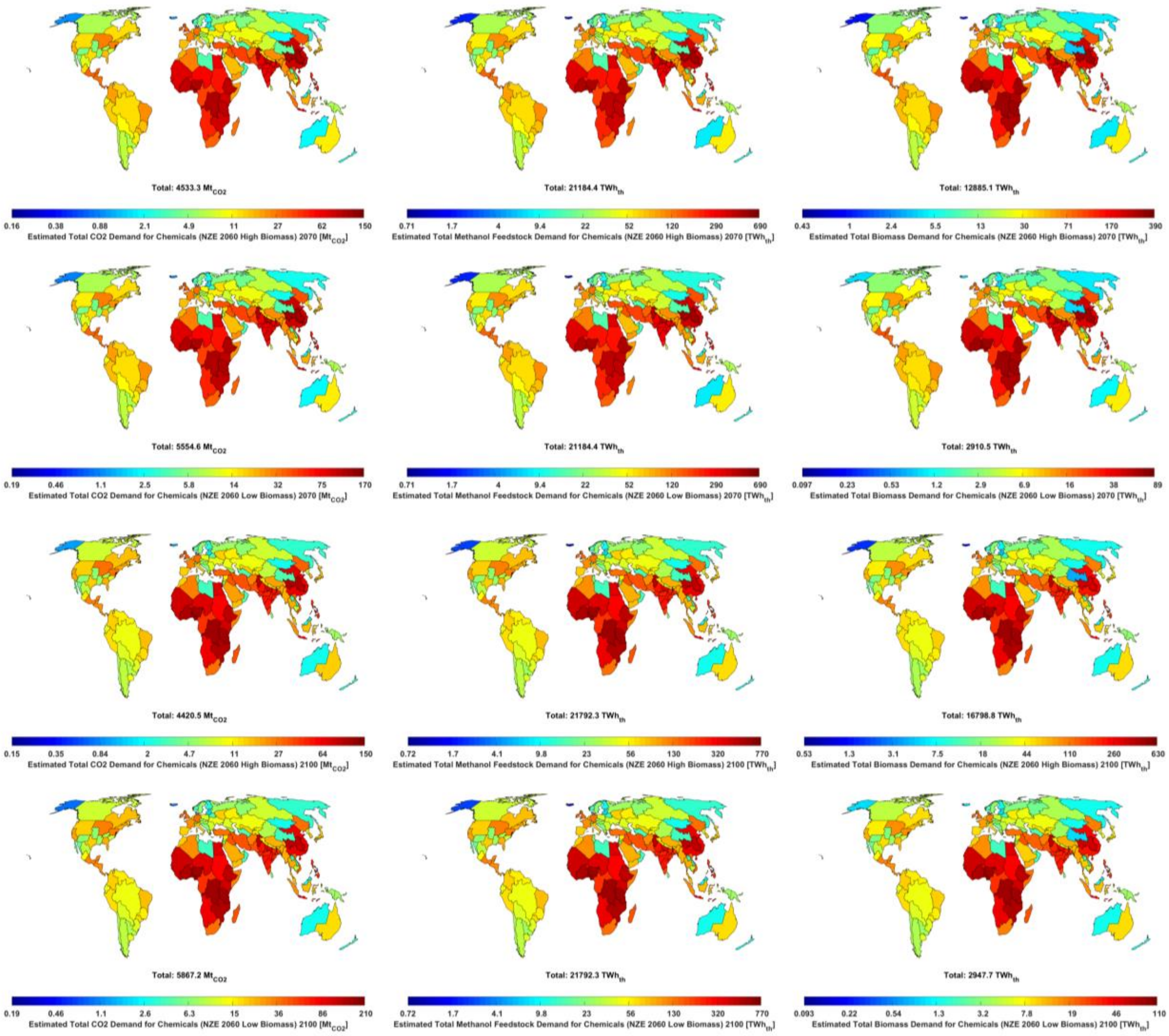


**Figure S30.** Total $CO_2$ (left), methanol feedstock (middle), and biomass demands (right) in 2070 (top) and 2100 (bottom) for the NZE 2060H (top of each row) and NZE 2060L (bottom of each row).

## 4.4. Financial Results

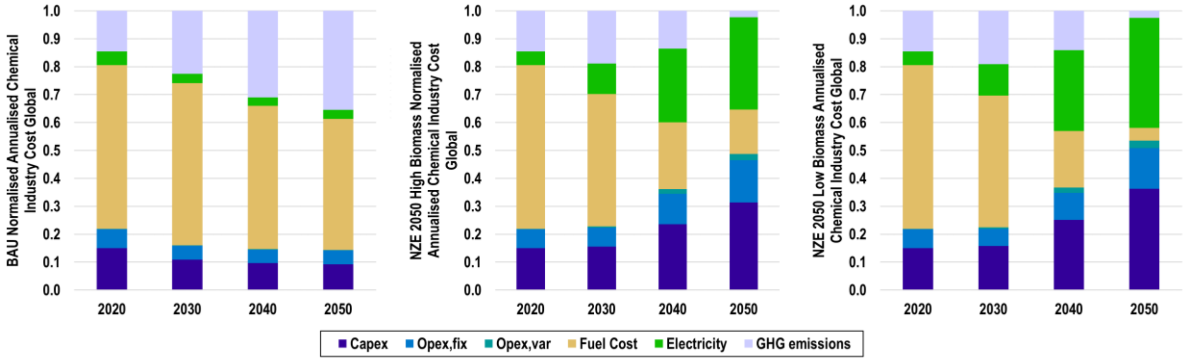


**Figure S31.** Normalised Global annualised costs for the BAU (top left), NZE 2050H (top right), and NZE 2050L (bottom) scenarios.

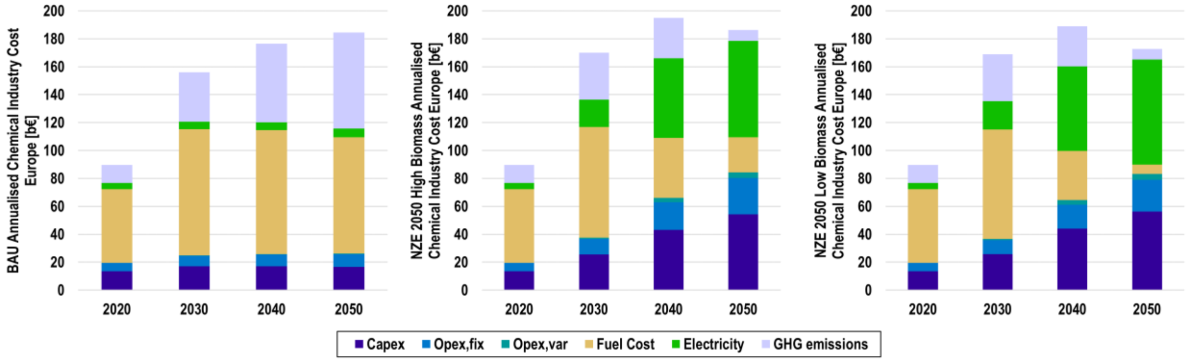


**Figure S32.** Annualised costs in Europe for the BAU (top left), NZE 2050H (top right), and NZE 2050L (bottom) scenarios.

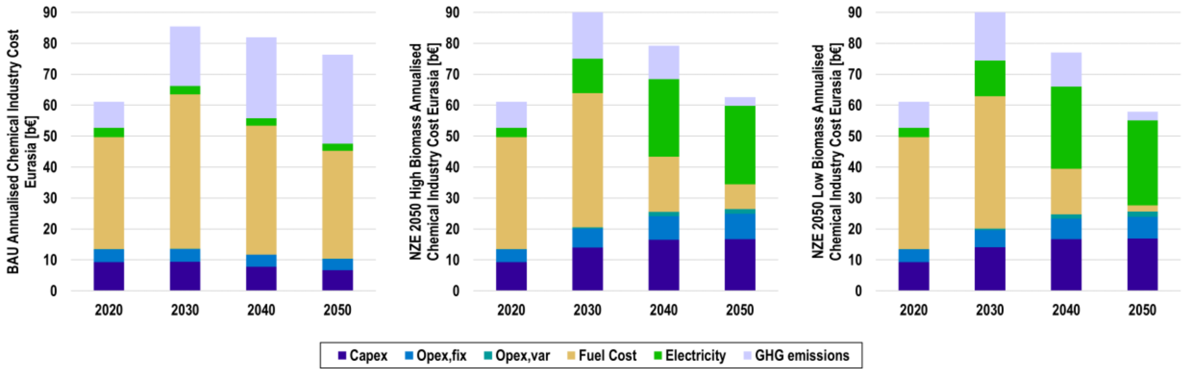


**Figure S33.** Annualised costs in Eurasia for the BAU (top left), NZE 2050H (top right), and NZE 2050L (bottom) scenarios.

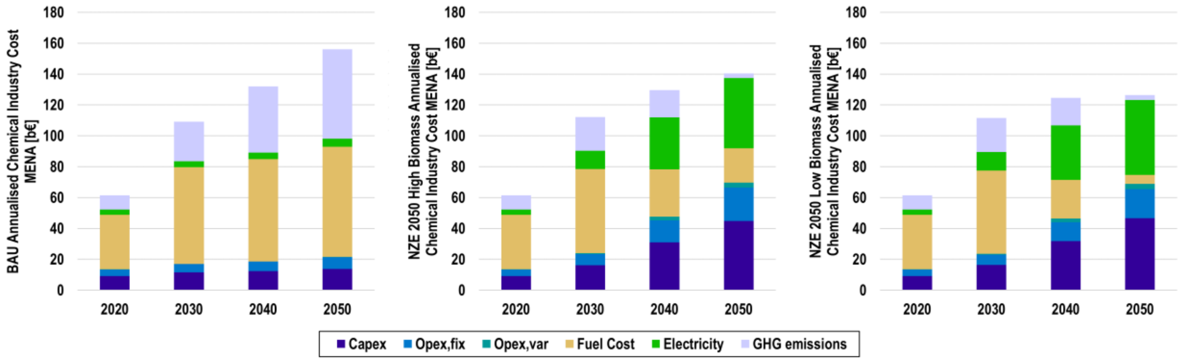


**Figure S34.** Annualised costs in the Middle East and North Africa (MENA) for the BAU (top left), NZE 2050H (top right), and NZE 2050L (bottom) scenarios.

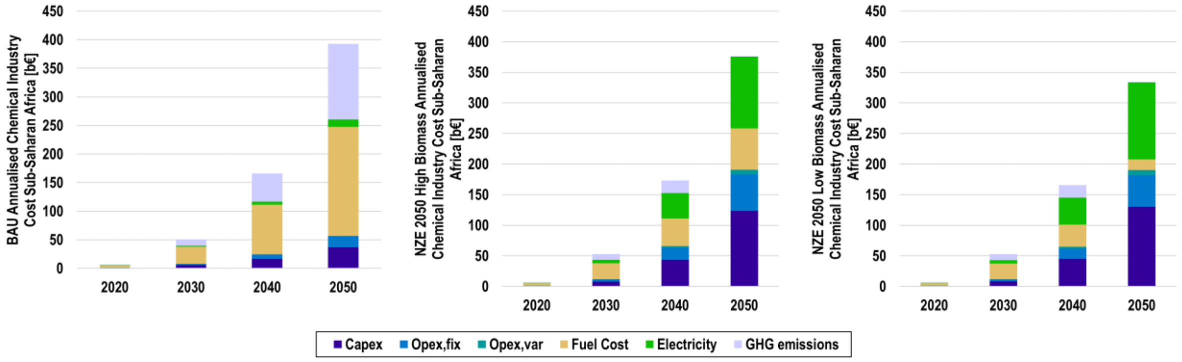


**Figure S35.** Annualised costs in sub-Saharan Africa for the BAU (top left), NZE 2050H (top right), and NZE 2050L (bottom) scenarios.

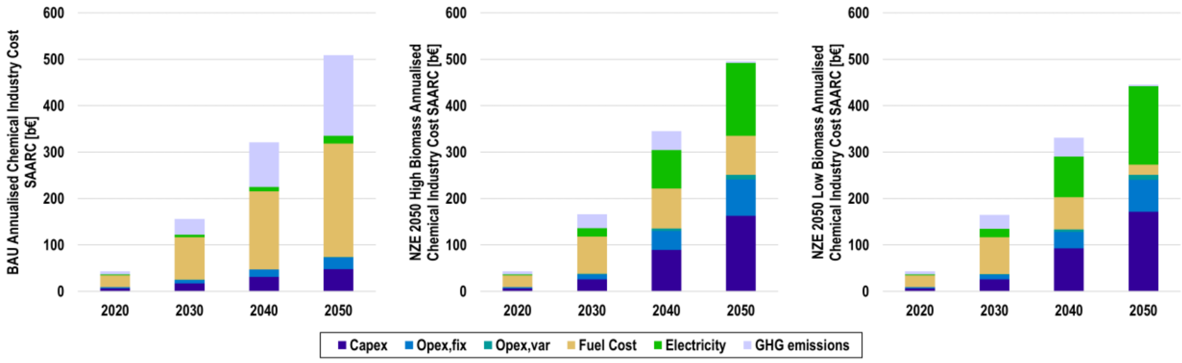


**Figure S36.** Annualised costs in the Southeast Asian Association for Regional Cooperation (SAARC) for the BAU (top left), NZE 2050H (top right), and NZE 2050L (bottom) scenarios.

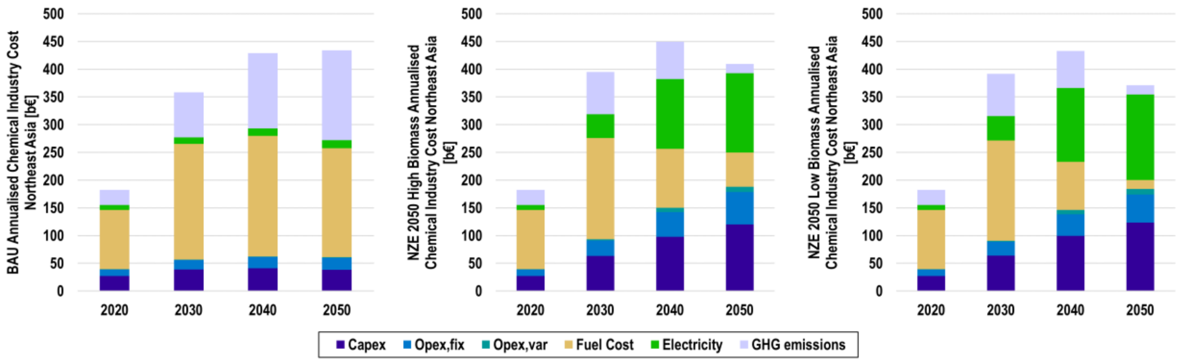


**Figure S37.** Annualised costs in Northeast Asia for the BAU (top left), NZE 2050H (top right), and NZE 2050L (bottom) scenarios.

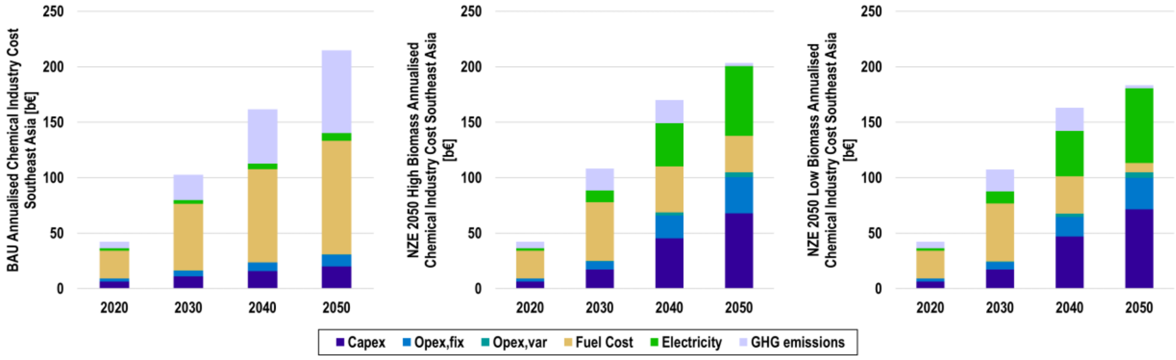


**Figure S38.** Annualised costs in Southeast Asia for the BAU (top left), NZE 2050H (top right), and NZE 2050L (bottom) scenarios.

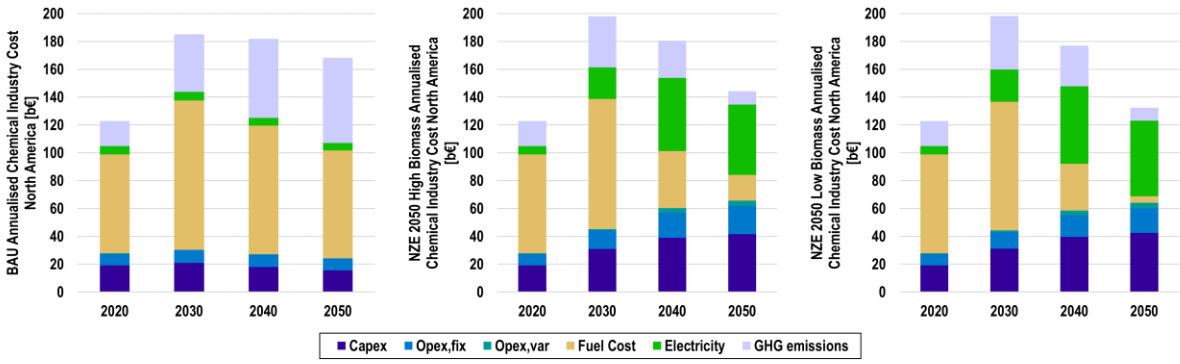


**Figure S39.** Annualised costs in North America for the BAU (top left), NZE 2050H (top right), and NZE 2050L (bottom) scenarios.

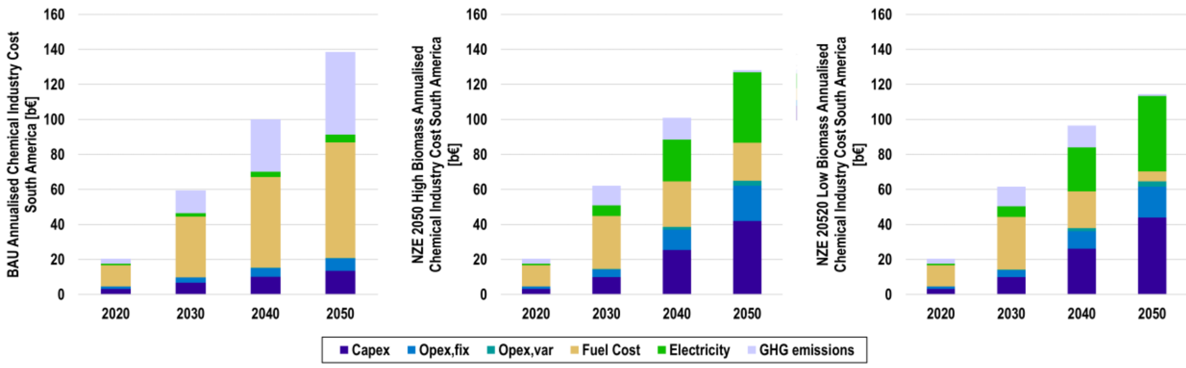


**Figure S40.** Annualised costs in South America for the BAU (top left), NZE 2050H (top right), and NZE 2050L (bottom) scenarios.

## 4.5. Chemical Feedstock Per Capita

### 4.5.1. BAU

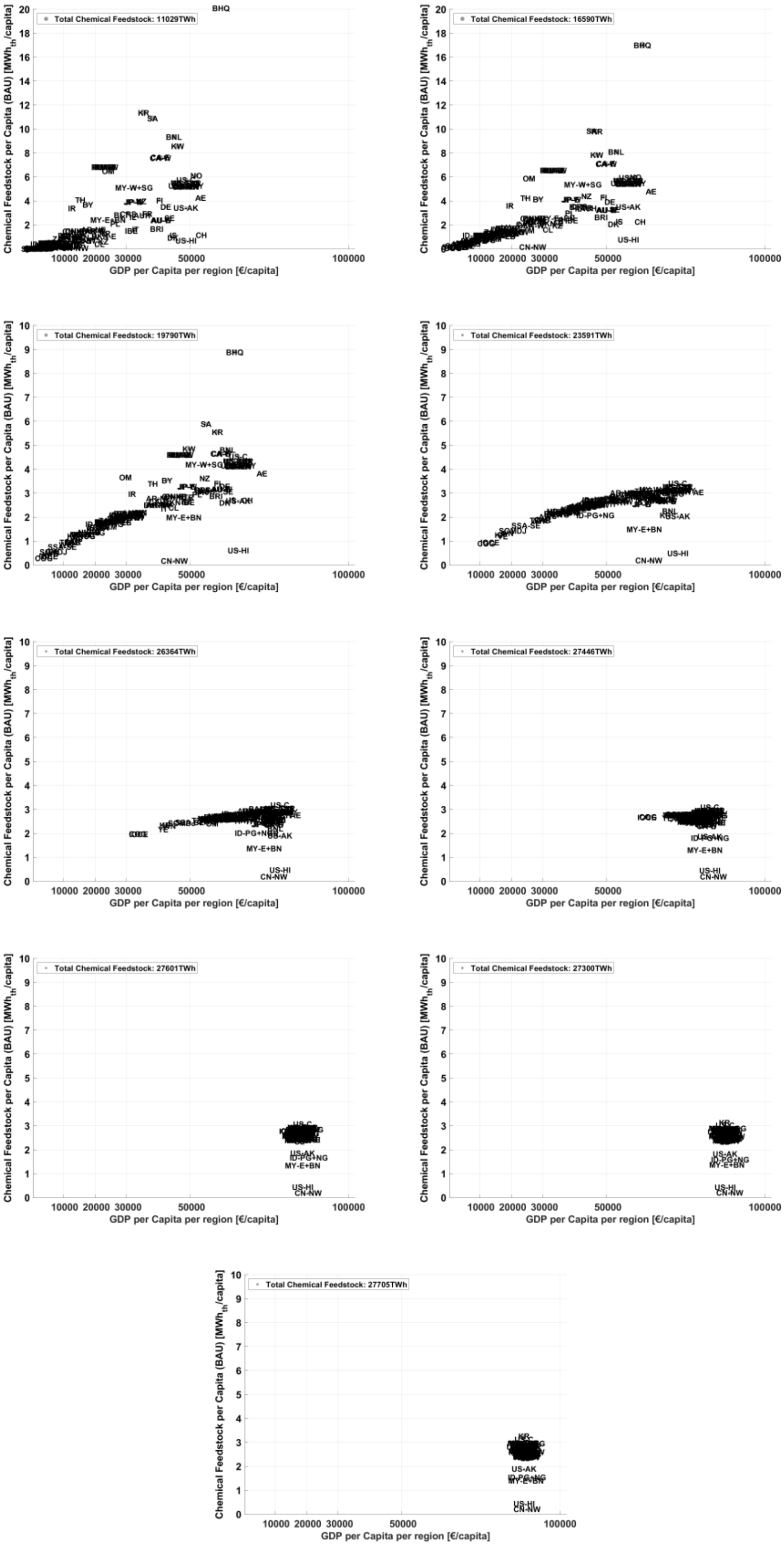


**Figure S41.** Chemical feedstock per capita over GDP per capita per global region for the BAU scenario in 2020 (top left), 2030 (top right), 2040 (second row left), 2050 (second row right), 2060 (third row left), 2070 (third row right), 2080 (fourth row left), 2090 (fourth row right), and 2100 (bottom)

## 4.5.2. NZE 2050

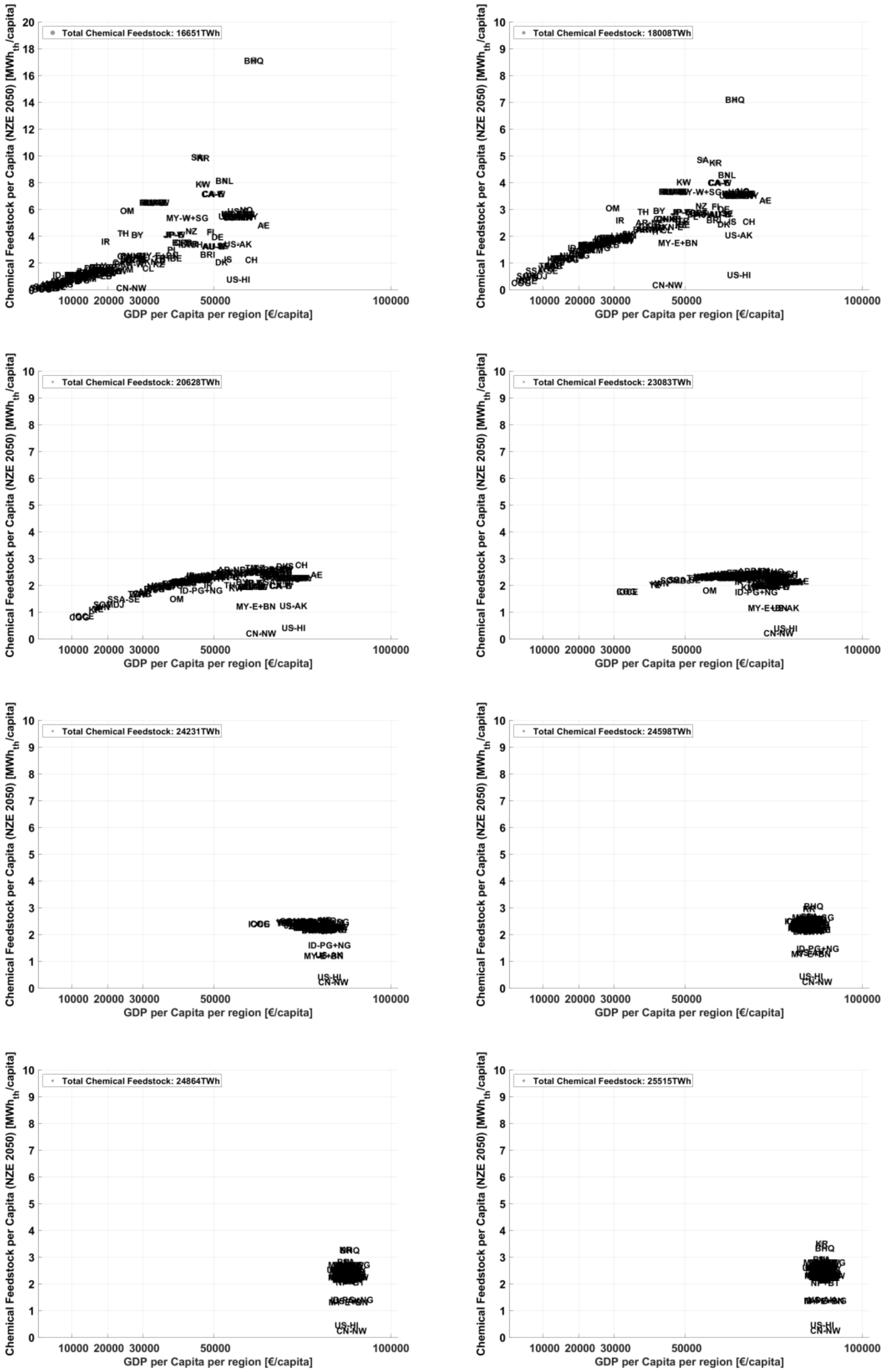


**Figure S42.** Chemical feedstock per capita over GDP per capita per global region for the NZE 2050 scenario in 2030 (top left), 2040 (top right), 2050 (second row left), 2060 (second row right), 2070 (third row left), 2080 (third row right), 2090 (bottom left), and 2100 (bottom right).

### 4.5.3. NZE 2040

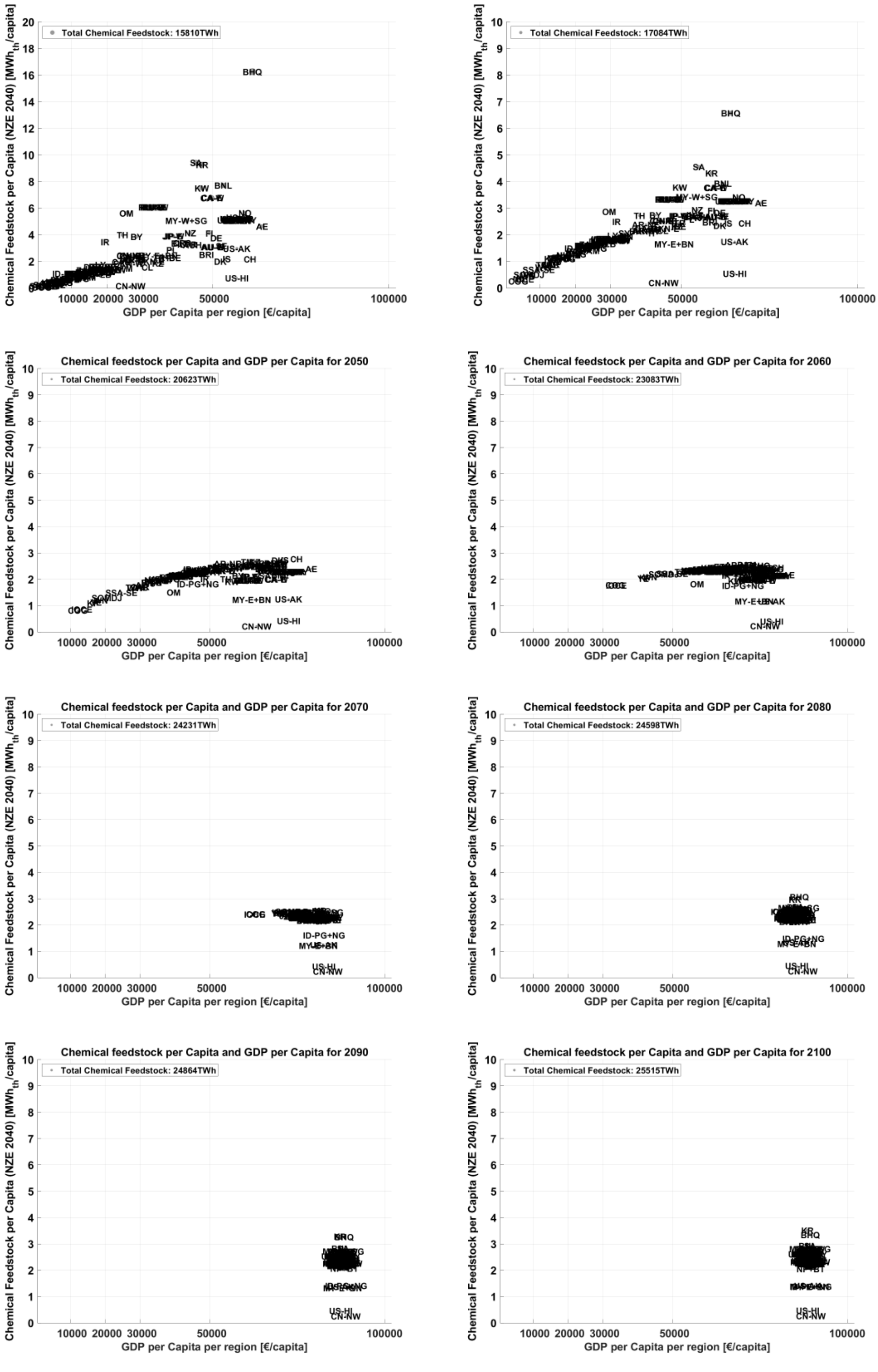


**Figure S43.** Chemical feedstock per capita over GDP per capita per global region for the NZE 2040 scenario in 2030 (top left), 2040 (top right), 2050 (second row left), 2060 (second row right), 2070 (third row left), 2080 (third row right), 2090 (bottom left), and 2100 (bottom right).

## 4.5.4. NZE 2060

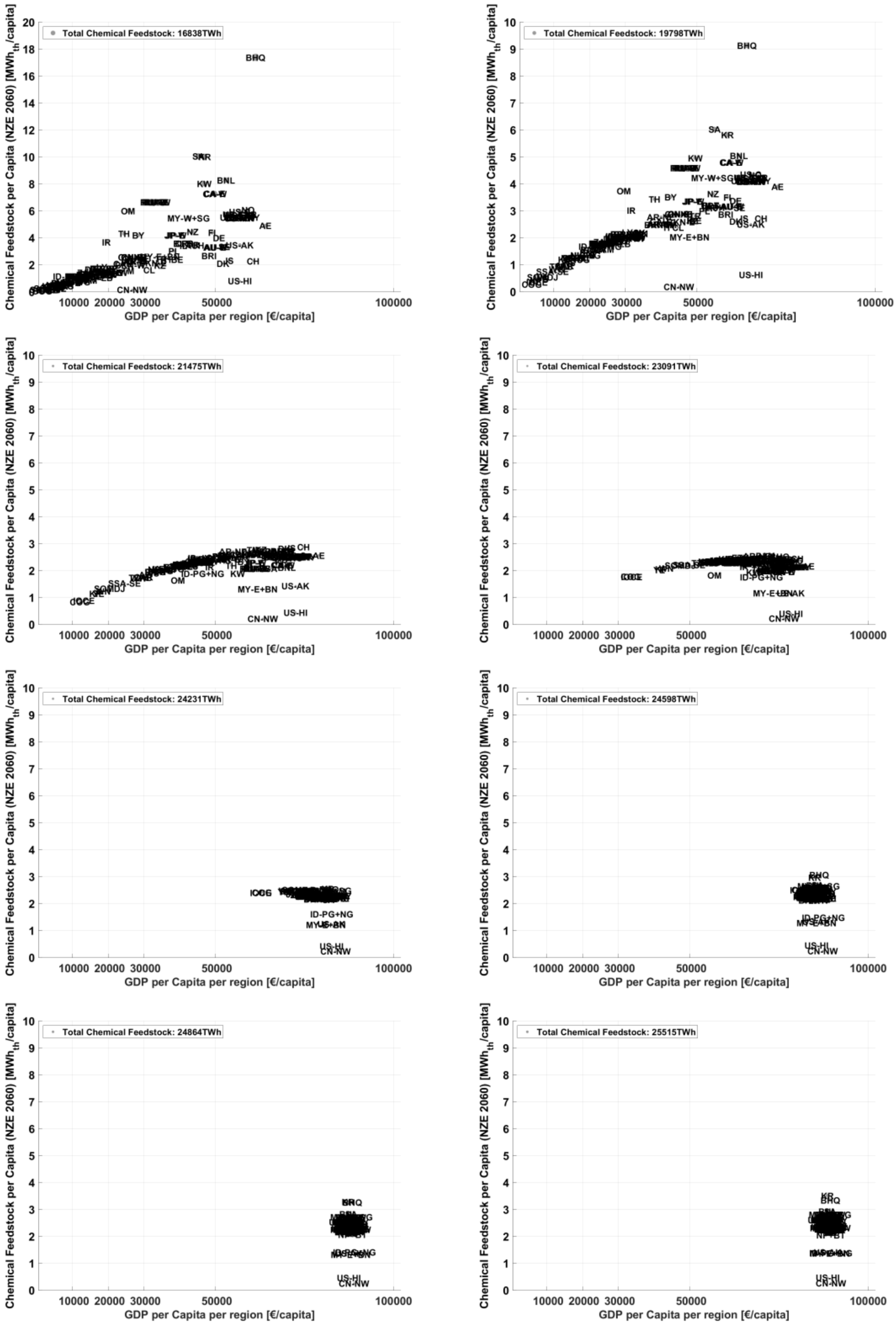


**Figure S44.** Chemical feedstock per capita over GDP per capita per global region for the NZE 2060 scenario in 2030 (top left), 2040 (top right), 2050 (second row left), 2060 (second row right), 2070 (third row left), 2080 (third row right), 2090 (bottom left), and 2100 (bottom right).

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