

In []:

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"""
3D Surface plot (Biprproduct vs Time and HCl(eq.))
- "Anilines in acid catalyzed amination with 4-ch
e"
- Hanne Svergj a
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"""

# Import required libraries
import numpy as np
import pandas as pd
from matplotlib import pyplot as plt
from scipy import interpolate

# Define the number of array splits for the 'bipr
n = 6

# Read the CSV file and select relevant columns
# Replace missing values with zero
df = pd.read_csv('svx_data.csv', delimiter=',', decimal='.',
                 usecols=['smolfrak', 'Bipr,prodHCl (eq.)'], dtype={
    'p.nan': 0})

# Split the 'biprod' column into 'n' equally size
# Transform the list of arrays into a NumPy array
bp = np.array([np.array_s(mf['biprod_b_nu(m),n'])])

# Define HCl equivalents and reaction time arrays
eq = np.array([0, 0.1, 0.5, 1, 3, 5])
t = np.array([0, 1, 2, 3, 4, 6])

# Create a 2D grid of HCl equivalents and reactio
T, EQ = np.meshgrid(t, eq)

# Define new, more detailed arrays for HCl equiva
tnew = np.linspace(0, 6, 100)
eqnew = np.linspace(0, 5, 100)

# Create a 2D grid of the new HCl equivalents and
tnew, eqnew = np.meshgrid(tnew, eqnew)

# Perform cubic interpolation of 'biprod' onto th
znew = interpola.griddata((t, eq), bp.flatten(), (tnew, eqnew),
                           method='cubic')

# Set the font style for the plot
plt.rcParams['font.family'] = 'Times New Roman'

# Define the color style for the 3D surface plot
cstyle = 'plasma'

# Create a new figure with 3D subplot
fig, ax = plt.subplots(subplot_kw={'projection': '3d'})

# Generate the 3D surface plot
hs = plt.plot_surface(tnew, eqnew, znew, cmap=cstyle, edgecolor='b',
                      linewidth=1, alpha=0.8, antialiased=True, shade=True)

# Add a color bar to the figure

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cbar = fig.colorbar(mappable=plt.cm.viridis,
                    ticks=plt.xticks(),
                    label='Side product (%)')

# Set ticks and label for the color bar
cbar.set_ticks([0, 5, 10, 15, 20, 25, 30])
cbar.set_label('Side product (%)')

# Set labels for the x, y, and z axes
ax.set_xlabel('Reaction time (h)')
ax.set_ylabel('HCl (eq.)')
ax.set_zlabel('Side product (%)')

# Set the limit for the z axis
ax.set_zlim(0, 30)

# Set the initial viewing angle
ax.view_init(30, -45)

# Turn off the grid
ax.grid(False)

# Adjust the padding around the plot
plt.tight_layout()

# Display the plot
plt.show()

# Save the figure as a high-resolution PNG file
fig.savefig('surfaceplot.mp4.png', box_inches=(10, 10))

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