

Comprehensive investigation of stoichiometry-structure-performance relationships in flexible polyurethane foams

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Table S1. The impact of isocyanate index on tensile strength – regression parameters and statistics.

| Regression parameters | | | Statistics | |
|------------------------------|---------------------|----------|-------------------------|----------|
| Regression type | linear | | Residual Sum of Squares | 732.48 |
| Equation | $y = a \cdot x + b$ | | Total Sum of Squares | 27992.00 |
| Parameter | a | b | R ² (COD) | 0.974 |
| Value | 509.524 | -357.524 | Adjusted R ² | 0.969 |
| Standard Error | 37.352 | 37.631 | Residual Standard | 12.10 |
| Lower confidence limit (95%) | 413.508 | -454.258 | | |
| Upper confidence limit (95%) | 605.540 | -260.790 | | |

Table S2. The impact of isocyanate index on compressive strength at 20% deformation – regression parameters and statistics.

| Regression parameters | | | Statistics | |
|------------------------------|-------------------|-------|-------------------------|---------|
| Regression type | non-linear | | Residual Sum of Squares | 36.02 |
| Equation | $y = a \cdot x^b$ | | Total Sum of Squares | 2176.17 |
| Parameter | a | b | R ² (COD) | 0.983 |
| Value | 16.916 | 6.899 | Adjusted R ² | 0.980 |
| Standard Error | 1.269 | 0.495 | Residual Standard | 2.68 |
| Lower confidence limit (95%) | 13.654 | 5.627 | | |
| Upper confidence limit (95%) | 20.179 | 8.171 | | |

Table S3. The impact of isocyanate index on compressive strength at 50% deformation – regression parameters and statistics.

| Regression parameters | | | Statistics | |
|-----------------------|-------------------|-------|-------------------------|----------|
| Regression type | non-linear | | Residual Sum of Squares | 264.88 |
| Equation | $y = a \cdot x^b$ | | Total Sum of Squares | 11580.18 |
| Parameter | a | b | R ² (COD) | 0.977 |
| Value | 36.979 | 7.147 | Adjusted R ² | 0.973 |

| | | | | |
|------------------------------|--------|-------|-------------------|------|
| Standard Error | 3.447 | 0.609 | Residual Standard | 7.28 |
| Lower confidence limit (95%) | 28.119 | 5.581 | | |
| Upper confidence limit (95%) | 45.839 | 8.713 | | |

Table S4. The impact of isocyanate index on tensile toughness – regression parameters and statistics.

| Regression parameters | | | Statistics | |
|------------------------------|---------------------|---------|-------------------------|--------|
| Regression type | linear | | Residual Sum of Squares | 1.58 |
| Equation | $y = a \cdot x + b$ | | Total Sum of Squares | 116.70 |
| Parameter | a | b | R ² (COD) | 0.986 |
| Value | 33.111 | -22.152 | Adjusted R ² | 0.984 |
| Standard Error | 1.735 | 1.748 | Residual Standard | 0.56 |
| Lower confidence limit (95%) | 28.652 | -26.644 | | |
| Upper confidence limit (95%) | 37.571 | -17.659 | | |

Table S5. The impact of isocyanate index on compressive toughness – regression parameters and statistics.

| Regression parameters | | | Statistics | |
|------------------------------|-------------------|-------|-------------------------|-------|
| Regression type | non-linear | | Residual Sum of Squares | 1.02 |
| Equation | $y = a \cdot x^b$ | | Total Sum of Squares | 43.62 |
| Parameter | a | b | R ² (COD) | 0.977 |
| Value | 2.122 | 7.510 | Adjusted R ² | 0.973 |
| Standard Error | 0.214 | 0.650 | Residual Standard | 0.45 |
| Lower confidence limit (95%) | 1.572 | 5.838 | | |
| Upper confidence limit (95%) | 2.671 | 9.182 | | |

Table S6. The impact of isocyanate index on glass transition temperature – regression parameters and statistics.

| Regression parameters | | | Statistics | |
|------------------------------|---------------------|---------|-------------------------|--------|
| Regression type | linear | | Residual Sum of Squares | 6.00 |
| Equation | $y = a \cdot x + b$ | | Total Sum of Squares | 469.33 |
| Parameter | a | b | R ² (COD) | 0.987 |
| Value | 66.429 | -48.557 | Adjusted R ² | 0.985 |
| Standard Error | 3.380 | 3.404 | Residual Standard | 1.09 |
| Lower confidence limit (95%) | 57.742 | -57.309 | | |
| Upper confidence limit (95%) | 75.115 | -39.806 | | |