Selective Reduction of Phenolic Compounds

Dinah Winter, Maria Cashmore, Martin Coleman, Graham Errington and Peter White
Background

**Phenolic compounds** are predominately associated with the **particulate phase** of smoke.

Primary purpose of **cellulose acetate (CA) filters** is the **reduction of particulate smoke yields**.

**Particulate phase** constituents are generally removed **in proportion to the tar filtration (removal) efficiency**.
Filtration (Removal) Efficiencies

The filter efficiency \( (E) \) for any smoke constituent is defined as:

\[
(E) = 100\% \left(1 - \frac{D}{A}\right)
\]

where: \( D \) is the yield of smoke constituent from the cigarette with a filter

\( A \) is the ‘available’ yield from the tobacco column with a plastic insert in place of a filter
Selective Filtration

Cellulose acetate shows a selective filtration for phenol. It is removed at a rate greater than the NFDPM removal efficiency. The selectivity index is given by:

\[ S_X = \frac{(1 - E_{NFDPM})}{(1 - E_X)} \]

- \( S_X \) = Selectivity index
- \( E_{NFDPM} \) = Filtration efficiency for NFDPM
- \( E_X \) = Filtration efficiency for component x
Introduction

- Previous work has shown that differences in the selective filtration of phenol, \( m + p \) cresol, \( o \)-cresol between cigarette designs were due to differences in cellulose acetate filter parameters.

- To gain a better understanding of how particular filter parameters might impact on the selective filtration of particular phenolic compounds a more detailed study was undertaken with Eastman Chemical Company.
Cellulose Acetate Study – Phase 1

2 level full factorial design

3 factors: 
- Length (mm)
- Tow weight (mg)
- Triacetin Level (%)

Tobacco: Virginia lamina
Constant column length

Responses: NFDPM, Phenol, o,p,m cresols, hydroquinone, catechol, resorcinol
## Factor Levels

<table>
<thead>
<tr>
<th>Factor</th>
<th>Units</th>
<th>Low Level</th>
<th>High Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filter Length</td>
<td>mm</td>
<td>22</td>
<td>42</td>
</tr>
<tr>
<td>Tow Weight*</td>
<td>mg</td>
<td>604</td>
<td>769</td>
</tr>
<tr>
<td>Triacetin</td>
<td>%</td>
<td>0</td>
<td>12</td>
</tr>
</tbody>
</table>

*Refers to 132 mm CA filter rod
All filters were 24.45mm circumference
Tow items were matched for NFDPM filtration efficiencies per mm of filter length
NFDPM Filter Efficiency (%) Cube Plot

Cube Plot for NFDPM Filtration Efficiency (%)
### Important Filtration Efficiency Factors

<table>
<thead>
<tr>
<th>Smoke Component</th>
<th>Filter Length</th>
<th>Triacetin Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>NFDPM</td>
<td>√</td>
<td></td>
</tr>
<tr>
<td>Phenol</td>
<td>√</td>
<td>√</td>
</tr>
<tr>
<td>o-cresol</td>
<td>√</td>
<td>√</td>
</tr>
<tr>
<td>m-cresol</td>
<td>√</td>
<td>√</td>
</tr>
<tr>
<td>p-cresol</td>
<td>√</td>
<td>√</td>
</tr>
<tr>
<td>Catechol</td>
<td>√</td>
<td></td>
</tr>
<tr>
<td>Resorcinol</td>
<td>√</td>
<td></td>
</tr>
<tr>
<td>Hydroquinone</td>
<td>√</td>
<td></td>
</tr>
</tbody>
</table>

Significant at 90%
Selectivity Index

\[ S_X = \frac{(1 - E_{NFDPM})}{(1 - E_x)} \]

- \( S_X \) = Selectivity index
- \( E_{NFDPM} \) = Filtration efficiency for NFDPM
- \( E_x \) = Filtration efficiency for component \( x \)

Davis, H and George, W., *Beitrage zur Tabakforschung*, 3,3 (1965) p203
## Selectivity Index & Filter Length

<table>
<thead>
<tr>
<th>Analyte</th>
<th>Triacetin (%)</th>
<th>Selectivity Index $S_x$</th>
<th>Filter Length (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phenol</td>
<td>0</td>
<td>1.75</td>
<td>2.47</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>2.35</td>
<td>5.22</td>
</tr>
<tr>
<td>o-cresol</td>
<td>0</td>
<td>1.51</td>
<td>1.69</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>1.98</td>
<td>3.41</td>
</tr>
<tr>
<td>Catechol</td>
<td>0</td>
<td>1.05</td>
<td>0.98</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>0.99</td>
<td>0.95</td>
</tr>
</tbody>
</table>
Estimating Phenol Filtration Efficiency

- **Estimate** phenol efficiency for **42mm** filter based on:

  22 mm filter at **12%** triacetin with $S_x = 2.35$

\[
(1 - Ex) = \frac{(1 - .63)}{2.35}
\]

- $Ex = 0.84$ giving an phenol filtration efficiency = **84%**

- Actual measured phenol filtration efficiency = **93%**
Modified Selectivity Index

\[ S_X = \frac{(1 - E_{NFDPM})}{(1 - E_X)} \]

To account for filter length:

\[ S'_X = \frac{\ln(1 - E_X)}{\ln(1 - E_{NFDPM})} \]

\( S_X \) = Selectivity index

\( E_{NFDPM} \) = Filtration efficiency for NFDPM

\( E_X \) = Filtration efficiency for component x
Modified Phenol Filtration Efficiency

- **Estimate** phenol efficiency for 42mm filter based on:
  - 22 mm filter at 12% triacetin with $S_x = 2.35$

- Predicted value of phenol filtration efficiency = 92%

- Actual value = 93%
Selectivity Index Comparisons

<table>
<thead>
<tr>
<th>Analyte</th>
<th>Triacetin (%)</th>
<th>$S_x$</th>
<th>$S'_x$</th>
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<tr>
<td></td>
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Conclusion

- Using tow items with matched NFDPM filtration efficiencies, the key factors influencing phenolic filtration efficiencies were:

  Filter length (mm)
  Triacetin (%)

- A modified equation for Selectivity has been proposed to account for filter length.

- Improved agreement between estimated and actual filtration efficiencies have been obtained for phenol and several other phenolic compounds.

- Further studies are required to assess the robustness of this approach.
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