Updating the Regulatory Compliance Assistance Program (RCAP) Tool to Improve TRI Reporting for the Polyurethane Industry

Session: Advances in TRI Data Reporting and Collection

Shen Tian, P.E.
EHS Engineer
Covestro, LLC

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Outline

- Introduction to the ACC CPI RCAP Tool
- Challenges in MDI and TDI emission reporting
- Updates made to the 2012 RCAP tool
- 2016 Tool validation: flexible foam as an example
- 2016 Tool illustration

ACC CPI RCAP Tool

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CPI Launches Expanded Regulatory Compliance Assistance Program for MDI Emissions

Contact: Marie Francis (202) 249-6514
Email: Marie_Francis@americanchemistry.com

Interactive tool has more options for calculating emissions for July 1 annual deadline

WASHINGTON (May 3, 2013) - The Center for the Polyurethanes Industry (CPI) of the American Chemistry Council (ACC) has expanded its Regulatory Compliance Assistance Program (RCAP) by upgrading the interactive tool designed to help manufacturers, processors and other users of diphenylmethane diisocyanate (MDI) and polymeric MDI (PMDI) in calculating emissions. This tools aids users in complying with mandatory reporting obligations to the U.S. Environmental Protection Agency (EPA) by estimating emissions from typical process applications and activities. Users who exceed the threshold limits set by EPA are required to submit a Form A or Form R by July 1st each year to EPA and the designated state agency.

Reportable Diisocyanates

CAS #/Category #	Chemical Name
584-84-9	2,4-TDI
91-08-7	2,6-TDI
26471-62-5	TDI mixed isomers
N 120	Diisocyanates (20 chemicals including MDI)

Challenges in MDI/TDI Emission Reporting

Assumes worst case scenarios

Over reporting in TRI and air permit application

- Saturated MDI/TDI in exhaust air
- Does not include chemical reactions

Challenges imposed upon industry

- Disproportionate regulatory compliance burden for small business
- Reputation management impact (UMass Toxic 100 Air Polluters Index)
- Higher ranking in EPA's chemical prioritization process (New TSCA)

Not applicable for MDI/TDI applications

- Existing tool is not customized for MDI/TDI applications
- Updated emission tool needs to be based on fundamental chemistry and physics

Certain modules in the previous version are not consistent with EPA emission reporting guidance

Lack of transparency in emission estimate algorithm selection and literature references

Updates Made to the 2012 RCAP Tool

Emission estimate algorithm	• Followed EPA reporting guidance for specific processes/applications • Avoided unnecessarily conservative assumptions • Added generic reaction rate of MDI/TDI, thus reducing reportable emissions
Tool interface and coding	• Added guidance, references and transparent modeling algorithms • Classified MDI/TDI application based on the fundamental emission mechanisms (e.g., close vs. open process) • Reduced the complexity in the application module selection • Increased programming efficiency
Potential benefits of the updated tool	• More accurate emission reporting • Cost saving (external consulting, testing, compliance) • Consistent reporting for the industry

Model Testing and Validation

Recruited volunteer testers from customers and trade associations: all positive feedbacks so far

Compared modeling results with field measurements for flexible foam (e.g., mattress): significant improvements on reportable TDI emissions

More application specific reaction rates to be added

Tool Validation: TDI Flexible Foam

Compare TDI emissions between modeled and measured data

- 2012 TDI RCAP tool assumes exhaust air is saturated with TDI vapor
- Stack monitoring results
- 2016 RCAP tool with EPA emission algorithm

Method	Total TDI Emitted before carbon filtration	
	Plant A (lb. in a 1-hr run)	Plant B (lb. in a 2-hr run)
2012 RCAP	15.2 (at 72 °F)	118 (at 90 °F)
Measured (stack testing)	0.09	0.20
2016 RCAP	0.65	1.59

Picture source: http://www.futureonehomes.com/mattress-foam-for-a-comfortable-mattress/

Tool Illustration

- Choose the module
- Understand the emission algorithm
- Collect production related data
- Use default values or collect customized data

Tool Overview

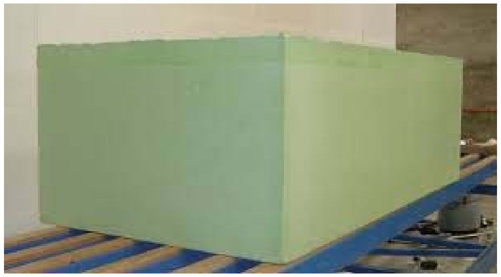
Group	Worksheet	Description
A. Group of administrative and application wide worksheets	A1 Overview	Home Page
	A2 Glossary	Glossary of abbreviations and terms
	A3 Links	List of links to online references
	A4 Guidance	Guidance for which calculation methods to use for which operations
M. Group of worksheets for Estimating Releases of MDI and PMDI	M1 Tank	Tank Filling and Storage emissions estimate for working and storage losses
	M2 Fugitive_Monitoring Data	Fugitive emissions calculated from monitoring data
	M3 Fugitive_Equipment Leaks	Overview page of equipment leaks modules
	M3a Fugitive_Equipment Leaks_No SV	Estimate fugitive emissions when no SV is available
	M3b Fugitive_Equipment Leaks- SV is Zero	Estimate fugitive emissions when SV is zero
	M3c Fugitive_Equipment Leaks_SV is not zero	Estimate fugitive emissions when SV is not zero
	M4 Enclosed Process_Overview	Overview page of the enclosed processes
	M4a Enclosed Process_Weight	Estimate emission when material weight is known
	M4b Enclosed Process_Volume	Estimate emission when container/cavity volume is known
	M5 Open Process	Overview page of the open processes and calcuate the reaction rate
	M5a Open Process	Estimate emission from open process with the consideration of reaction rate
	M5b Open Process Oven	Estimate emission from drying oven after the open process
	M6 Exhaust Air-Measured	Estimate emission from measured concentration in exhaust air
	M6S Exhaust Air_Saturated	Estimate emission from exhaust air assuming saturated with MDI vapor
	M7 Binding Agent	Estimate emission from application using MDI/pMDI as binding agent
	M8 Spill	Estimate emission from spill
	M9 Spray Coating	Estimate particle phase emission from spray coating process
	M9a Spray Coating_Oven	Estimate vapor phase emission from drying oven
	M9b Spray Coating_Air Dry	Estimate vapor phase emission from air dry process
R - Reference Tables	R1 Reference Lookups	Collection of lookup administrative tables
	R2 Reference Tables	Collection of reference data tables such as vapor pressure of mercury, percent of composition for MDI/PMDI, and so forth
S - Summary	S1 Emissions Summary	Emission totals

Worksheet Selection Guidance

M4: Enclosed process may include the following applications:

- ❖Reaction Injection Molding (RIM)
- ❖Molded foam parts (automotive and furniture)
- ❖Cast elastomers (shoe soles, packaging, furniture)
- ❖Pour-in-place (appliance insulation, marine products)
- ❖Filling/mixing/blending in a closed vessel or container

M5: Open process may include the following applications:



- ❖Slabstock/bunstock
- ❖Laminate boardstock
- ❖Metal skin panels
- ❖Carpet backing/flooring/coating
- ❖Belt and tire cord
- ❖Bonded foam production
- ❖Spandex, lycra, elastin, etc.

M7: Using MDI as a binding agent, such applications may include:

- ❖Foundries and casters
- ❖Oriented strand board
- ❖Particle board
- ❖Sandwich panels

Picture source:
https://www.alibaba.com/product-detail/Rotary-Type-Automatic-Polyurethane-Single-Density_60197180499.html
http://www.appliedpolymers.com.au/products/typical-application/rigid-foam-slabstock/
http://info.cpm-industries.com/blog/bid/324839/Foundry-Tooling-Materials

Example: TDI Flexible Foam

Compare TDI emissions from flexible foam production

- 2016 RCAP tool with EPA emission algorithm;
- 2012 TDI RCAP tool: assume exhaust air is saturated with TDI vapor;
- Stack monitoring results.

Plant A:

Term	Quantity	Unit	Comment
A	8,300	ft^2	Enter surface area of product produced, do not include surface area not exposed to air, e.g., the bottom area of a foundry on conveyor or foam surface covered by other materials
t	1.0	hrs	Enter the estimated curing time (starting from mixing TDI with polyol and ending when the product is considered cured)
Air velocity over the product before curing (e.g., on a conveyor)	1.8	ft/sec	Enter value and select units (typical indoor velocity: 1-3 ft/s)
T_{open}	120.0	F	Enter temperature and select units: F, K, or C.
C_{form}	50	percent	Enter molar % of TDI in the formulation, 1-100, 100 if only TDI exists, weight % can be used if it is close to molar %
k_r	3.5	1/hr	Enter the estimated first order reaction rate of TDI with polyol, default value is 7.2/hr
η	0.0	percent	Exhaust filter efficiency, 0-100
L_{open}	**6.52E-01**	**lb**	Calculated TDI emissions considering reaction and filter

Example: TDI Flexible Foam

2016 version RCAP tool with EPA emission algorithm:

Plant B:

Term	Quantity	Unit	Comment	Data Set #
A	20,286	ft^2	Enter surface area of product produced, do not include surface area not exposed to air, e.g., the bottom area of a foundry on conveyor or foam surface covered by other materials	1
t	1.0	hrs	Enter the estimated curing time (starting from mixing TDI with polyol and ending when the product is considered cured)	1
Air velocity over the product before curing (e.g., on a conveyor)	1.8	ft/sec	Enter value and select units (typical indoor velocity: 1-3 ft/s)	1
T_{open}	120.0	F	Enter temperature and select units: F, K, or C.	1
C_{form}	50	percent	Enter molar % of TDI in the formulation, 1-100, 100 if only TDI exists, weight % can be used if it is close to molar %	1
k_r	3.5	1/hr	Enter the estimated first order reaction rate of TDI with polyol, default value is 7.2/hr	1
η	0.0	percent	Exhaust filter efficiency, 0-100	1
L_{open}	**1.59E+00**	**lb**	Calculated TDI emissions considering reaction and filter	1

Key parameters:

1. Production rate
2. Foam surface temperature

Picture source:
http://www.virtualpu.com/newsletter1.php?id=551&login_part_from=latest_trends_patents&page_from=newsletter&doc_id=49803

Example: TDI Flexible Foam

2012 TDI RCAP tool: exhaust air is saturated with TDI vapor:

	Plant A	Plant B
Exhaust air temperature (°F)	72	90
Saturated TDI concentration (g/m^3)	0.1	0.25
Exhaust fan rate (CFM)	40,197	62,926
Total Emission (lb)	15.2	117.8

Typical TDI concentration from stack sampling: 0.35 mg/m^3 (90 °F)

Saturated TDI concentration: 250 mg/m^3 (90 °F)

~700 times higher if assume saturated concentration!

Picture source:
http://www.pufoamcuttingmachine.com/supplier-85169-foam-production-line

Example 2: Open Process (MDI)

Step 1: Estimate pseudo 1st order reaction rate

$$k_r = -\frac{\ln(\frac{R'}{100})}{\Delta t}$$

Term	Quantity	Unit
k_r	4.605170186	1/hr
R'	1	%
Δt	1	hr

Step 2: calculate emissions assuming a 1st order reaction

Term	Quantity	Unit	Comment	Data Set #
A	20,000,000	ft^2/yr	Enter surface area of product produced per year, do not include surface area which is not exposed to air, e.g., the bottom area of a foundry on conveyor or foam surface covered by other materials	1
t	1	hrs	Enter the estimated curing time (starting from mixing MDI/pMDI with polyol and ending when the product is considered cured)	1
Air velocity over the product before curing (e.g., on a conveyor)	1.8	ft/sec	Enter value and select units (typical indoor velocity: 1-3 ft/s)	1
T_{open}	68.0	F	Enter temperature and select units: F, K, or C.	1
% MDI in MDI/PMDI (K_{MDI})	50	percent	Enter molar % of 4,4' and 2,4' MDI monomer in MDI/PMDI, 1-100, weight % can be used if it is close to molar %. Contact supplier if not sure	1
C_{form}	50	percent	Enter molar % of MDI/PMDI in the formulation, 1-100, 100 if only MDI/pMDI exists, weight % can be used if it is close to molar %	1
k_r	3.6	1/hr	Enter the estimated first order reaction rate of MDI/pMDI with polyol, default value is 3.6/hr	1
η	0.0	percent	Exhaust filter efficiency, 0-100	1
				1
L_{open}	**3.17E-02**	**lb/yr**	Calculated MDI emissions considering reaction and filteration	1

Example 2: Open Process (MDI)

In the 2012 RCAP, since it does not consider reaction and assumes all exhaust air is saturated with MDI, the reportable emission is much higher!

Term	Quantity	Unit	Comment	Data Set #
Exhaust Airflow Rate	30,000.0	CFM	Enter velocity of blower operations	1
T_{sp} Exhaust Temperature	68.0	F	Enter temperature and select units: F, K, or C.	1
% MDI in MDI/PMDI	50	percent	Enter percentage MDI in MDI/PMDI.	1
C_f	50	percent	Enter percentage of MDI/PMDI in the total formulation.	1
Hours of operation per year	2,080	hrs/yr	Enter time of operations for the year.	1
				1
L_{annual}	**4.69E+00**	**lb/yr**	Calculated emissions of diisocyanates	1

Recall from last slide: annual emission of 20 million sq. ft. products is only 3.17×10^{-2} lb!

Emission depends on production rate, not the ventilation fan

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Thanks!

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place.

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