



 **BASF**

We create chemistry

Agnique® AMD 3 L

A sustainable, water-soluble solvent
for Industrial Formulators

Background

- Solvents have to fulfil increasingly demanding **environmental**, **health** and **safety** criteria, while achieving excellent **performance** and **quality** standards
- Widely used polar solvents like **NMP** (N-methyl-2-pyrrolidone), **NEP** (N-ethyl-2-pyrrolidone), **DMF** (dimethyl formamide) and **DMAc** (dimethyl acetamide) suffer from a dangerous labelling and are considered as SVHC (substance of very high concern)
- **Agnique® AMD 3 L** (N,N-dimethyl lactamide) is an established solvent for agro formulations. It is **label-free**, **bio-based**, **readily biodegradable** and **REACH registered**. Hence it fulfils all the needs as a sustainable solvent for technical applications.



Agnique® AMD 3 L

Characteristics

■ Properties

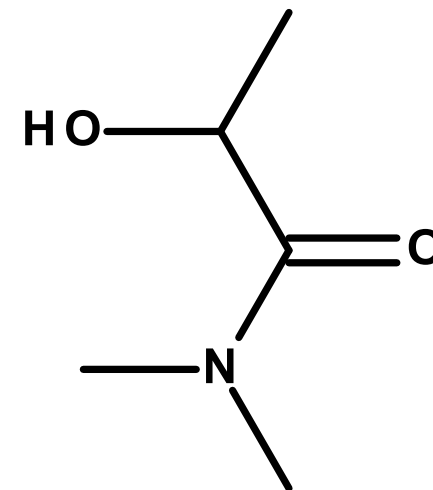
- ▶ Fully water soluble, protic amide
- ▶ Pour point: -60 °C
- ▶ Flash point: 103 °C
- ▶ Boiling point: 223 °C

■ Label free according to GHS

■ Readily biodegradable according to OECD 301

■ Bio-based (lactic acid from fermentation)

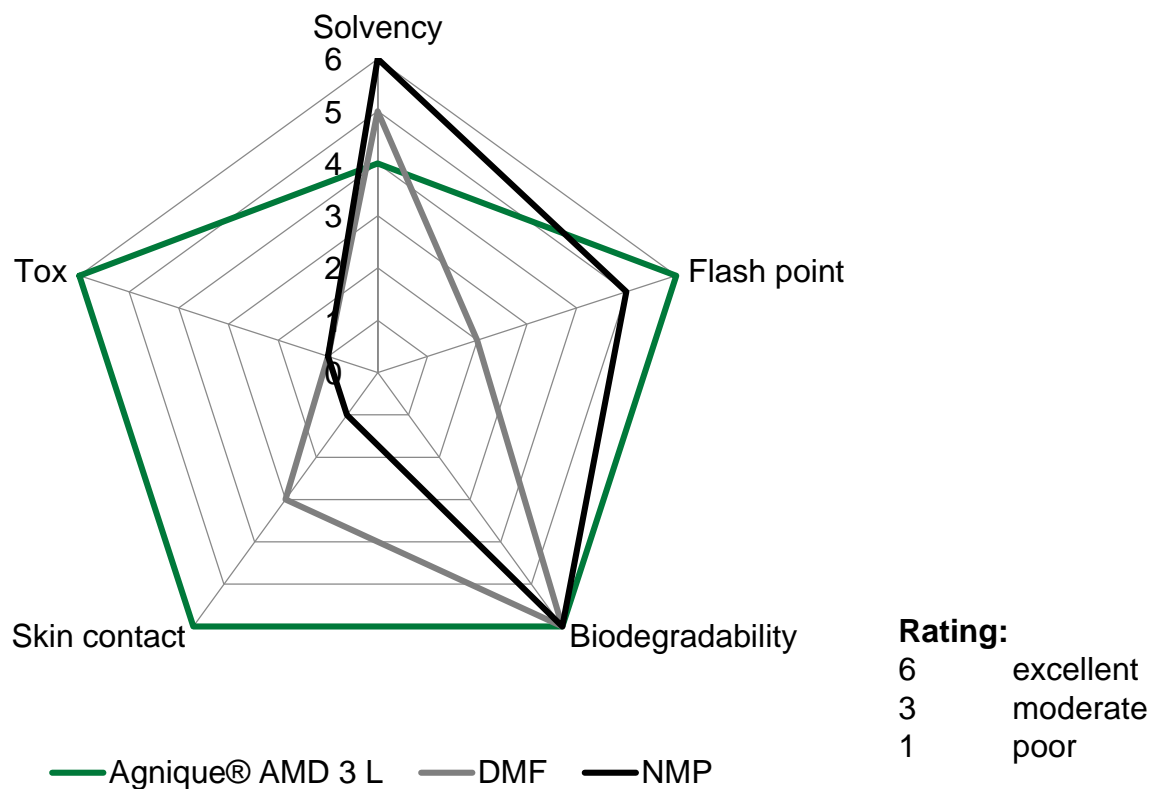
■ REACh and TSCA registered



Agnique® AMD 3 L

Comparison of Solvent Profile

Agnique® AMD 3 L combines very good solvency with superior safety and ecological performance



Agnique® AMD 3 L

Toxicological Evaluation (I)

Safety Aspect	Test Method	Test Result
Acute Oral Toxicity	OECD 423	>2000 mg/kg
Acute Inhalation Toxicity	OECD 403	>5 mg/L 4h
Acute Dermal Toxicity	OECD 402	>2000 mg/kg
Skin Irritation	OECD 404	Not irritating
Eye Irritation	OECD 405	Not irritating
Skin Sensitization	OECD 429	Not sensitizing
Repeated Dose Oral Toxicity	OECD 408	NOAEL = 200 mg/kg/d
Genetic Toxicity (Mutagenicity)	OECD 471 / 476 / 487	Negative
Developmental Toxicity (Teratogenicity)	OECD 414	NOAEL = 500 mg/kg/d

Agnique® AMD 3 L

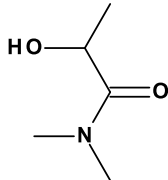
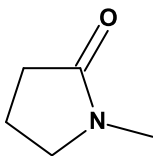
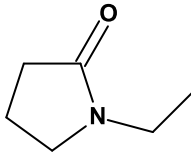
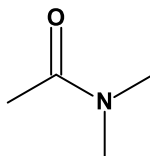
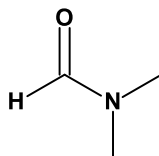
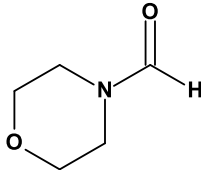





Toxicological Evaluation (II)

Safety Aspect	Test Method	Test Result
Acute Toxicity to Fish	OECD 203	LC50 > 100 mg/L
Acute Toxicity to Daphnia	OECD 202	EC50 > 100 mg/L
Reproduction Toxicity to Daphnia	OECD 211	NOEC >1mg/L
Toxicity to Algae and Cyanobacteria	OECD 201	EC50 > 100mg/L
Toxicity to Microorganisms	OECD 209	EC50 > 1000 mg/L
Toxicity to Soil Macroorganisms	OECD 207	NOEC > 1000 mg/kg
Toxicity to Terrestrial Plants	OECD 208	NOEC > 1000 mg/kg
Toxicity to Soil Microorganisms	OECD 216	NOEC < 62.5 mg/kg
Biodegradation	OECD 301 B	Readily biodegradable

AMD 3L has been intensively tested and does not bear any labelling

Agnique® AMD 3 L

Solvent Properties

Product	AMD 3L	NMP	NEP	DMAc	DMF	NFM
CAS No.	35123-06-9	872-50-4	2687-91-4	127-19-5	68-12-2	4394-85-8
Formula						
Classification	NONE					
SVHC ⁽¹⁾	no	SVHC	SVHC	SVHC	SVHC	So far none
m.p. / b.p. [°C]	-60 ⁽²⁾ / 223	-23 / 204	-75 / 212	-20 / 165	-61 / 152	21 / 244
Flash point [°C]	103	91	91	63	58	108
Water solubility	Miscible	Miscible	Miscible	Miscible	Miscible	Miscible
Vapor pressure 20°C [hPa]	< 0.1	0.32	0.18	3.30	3.56	0.20
Viscosity 20°C [mPa*s]	5.1	1.7	2.1	0.9	0.9	7.6

⁽¹⁾ Substances of Very High Concern

⁽²⁾ Pour point

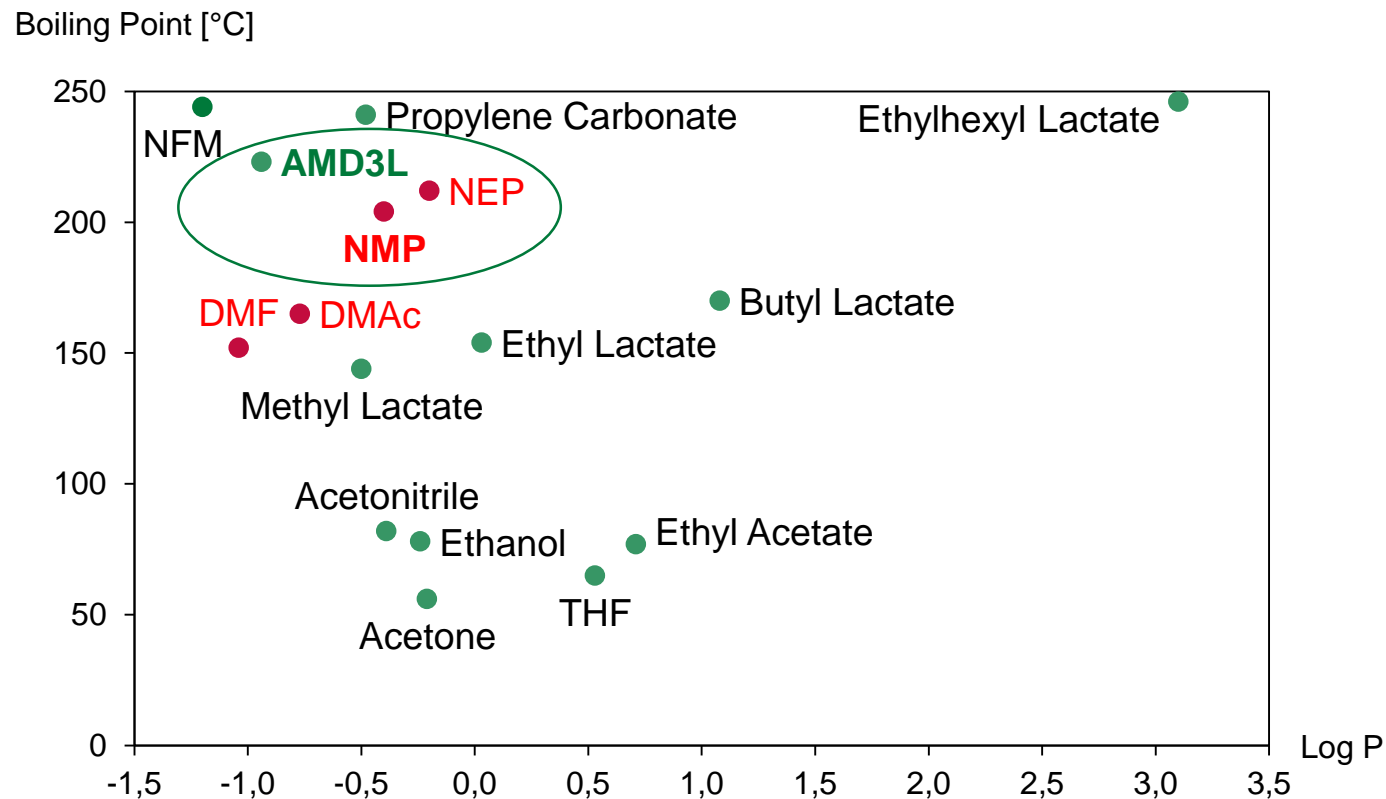
Agnique® AMD 3 L

Solubility Parameter

Product	AMD 3 L	NMP	NEP	DMAc	DMF	NFM
Hansen Solubility Parameters (HSP)						
Dispersion δ_d [MPa ^{1/2}]	18,4	18,0	18,0	16,8	17,4	21,9
Polar δ_p [MPa ^{1/2}]	12,9	12,3	12,3	11,5	13,7	14,4
Hydrogen Bonding δ_h [MPa ^{1/2}]	15,9	7,2	7,2	10,2	11,3	10,0
Partition Coefficient						
Log P (octanol/water)	-0,94	-0,40	-0,20	-0,77	-1,04	-1,20

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Boiling Point and Partition Coefficient (log P)

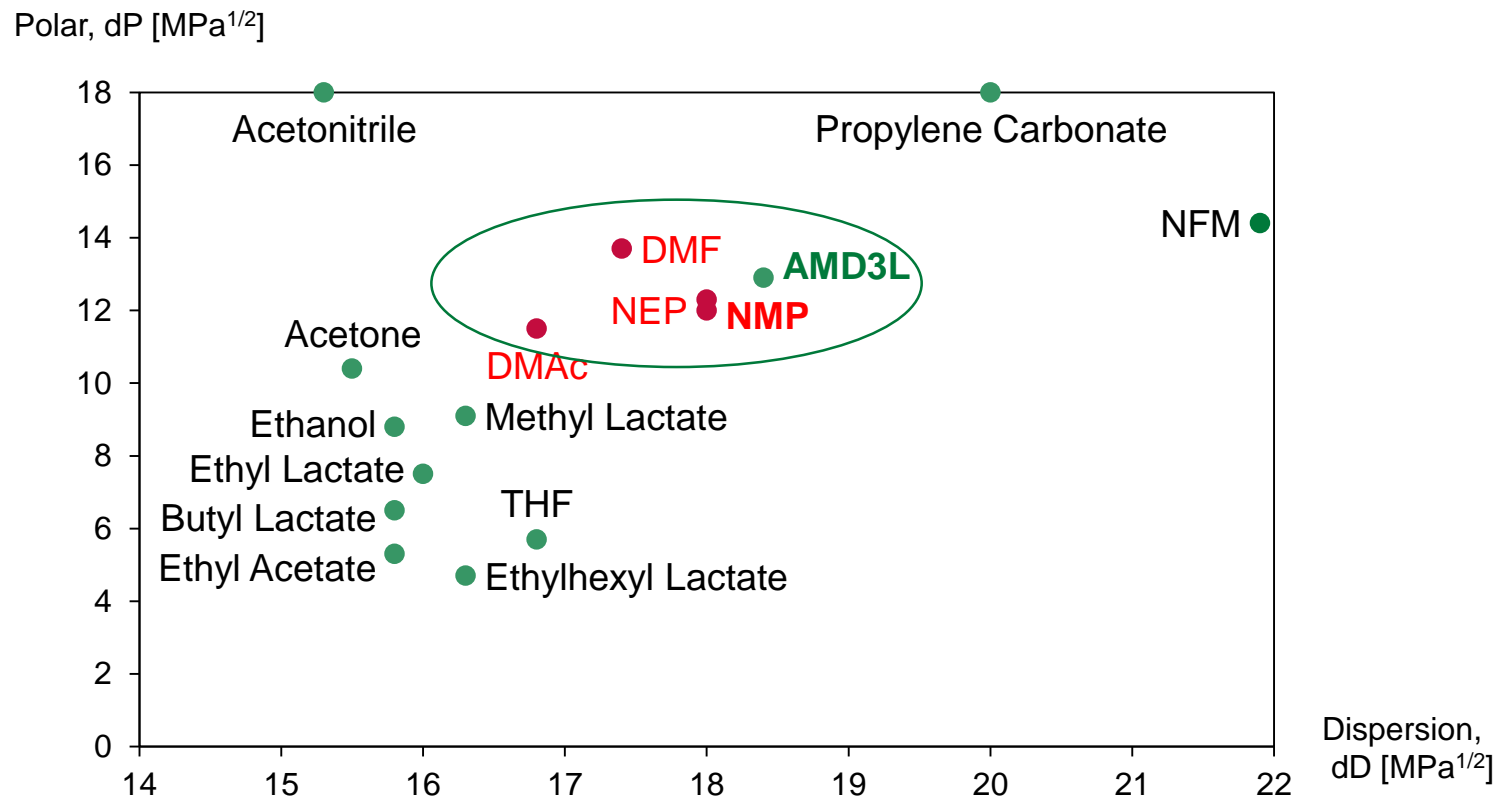


Boiling point and partition coefficient of AMD 3L are very close to NMP and NEP



Agnique® AMD 3 L

Hansen Solubility Parameter: Polar vs. Dispersion



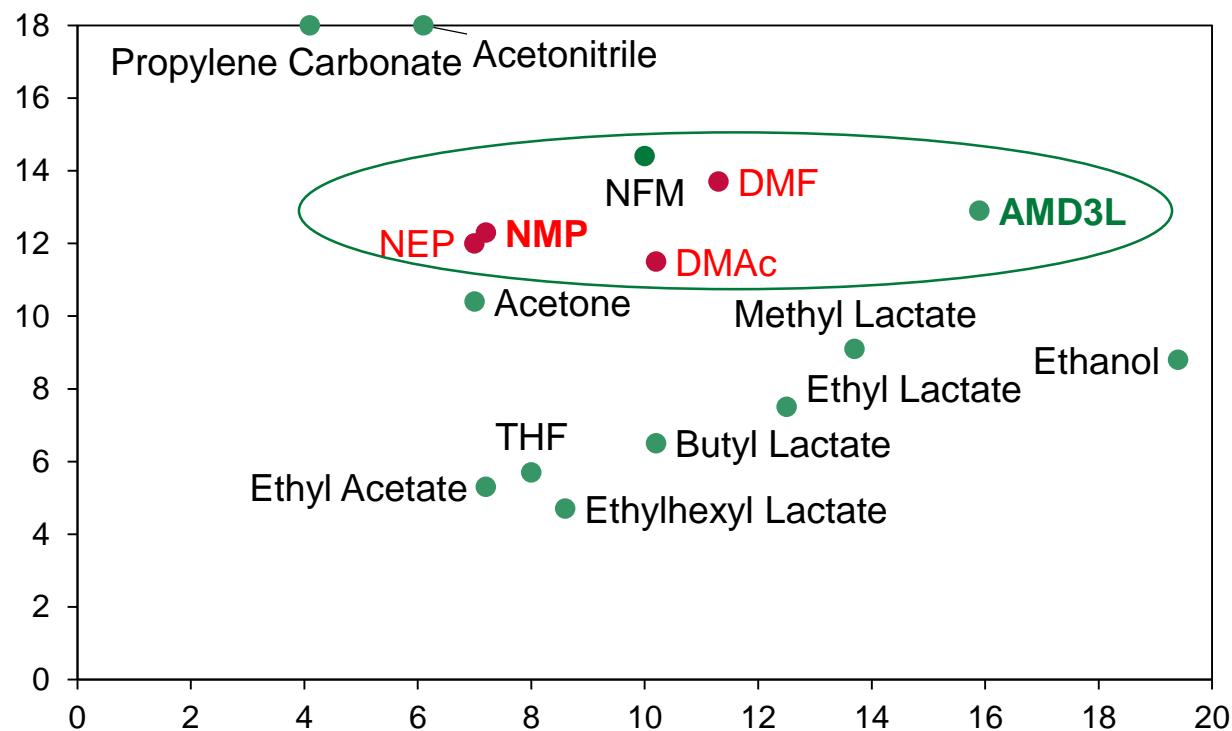
Hansen polar and dispersion parameter for AMD 3L are very close to NMP, NEP, DMF and DMAc



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Hansen Solubility Parameter Polar vs. Hydrogen Bonding

Polar, dP [MPa^{1/2}]



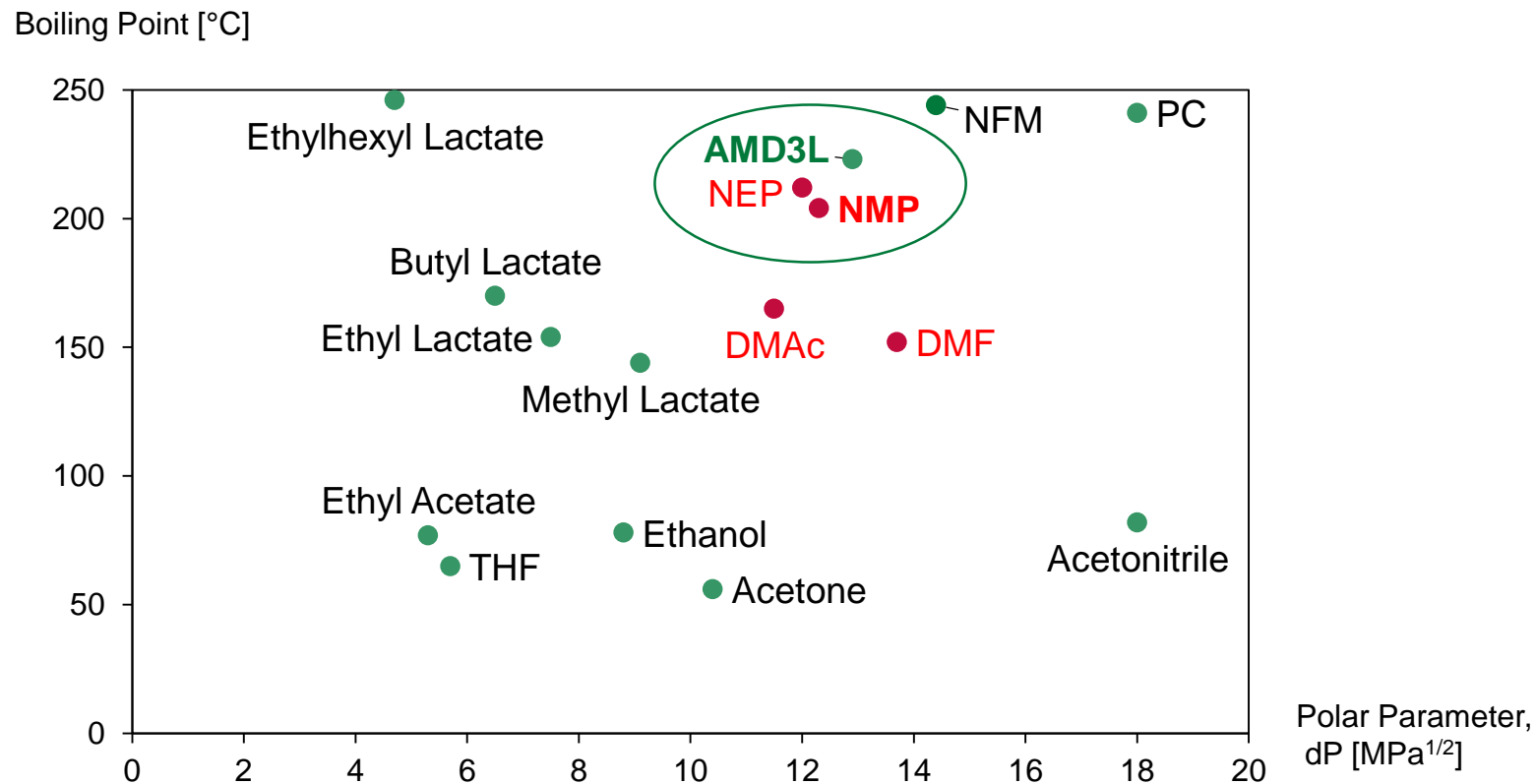
Hydrogen Bonding, dH [MPa^{1/2}]

Hydrogen bonding parameter of AMD 3 L is higher due to the protic nature



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Boiling Point vs. Hansen Polar Parameter

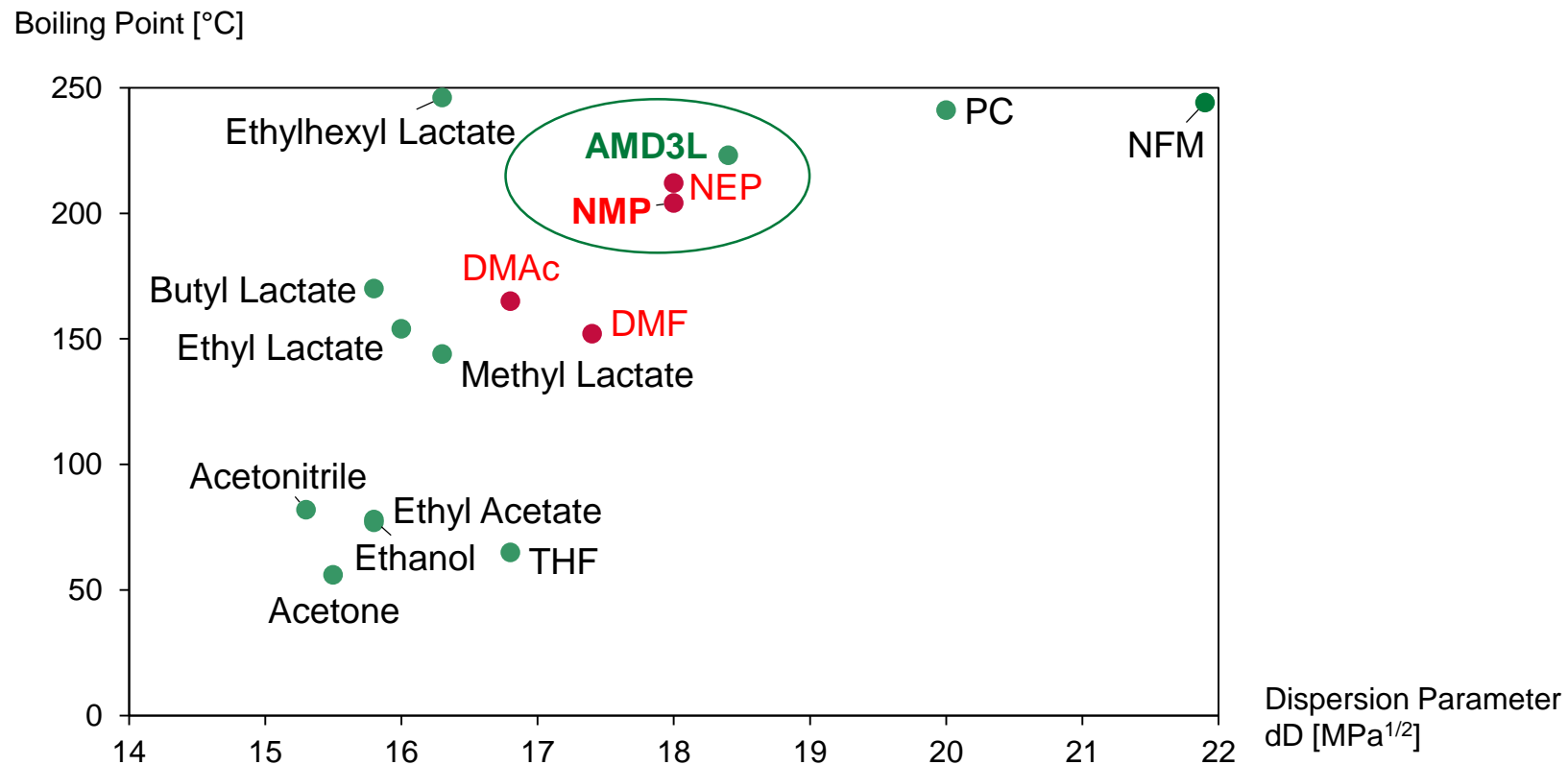


Boiling point and Hansen polar parameter of AMD 3 L are very close to NMP



Agnique® AMD 3 L

Boiling Point vs. Hansen Dispersion Parameter



Boiling point and Hansen dispersion parameter of AMD 3L are very close to NMP



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Applications

Current applications

- Agrochemical formulations
- Ultrafiltration membranes
- Solvent for coatings formulations
- Solvent for inks formulations
- Photoresist stripper for printed circuit boards
- Solvent for PU reactor cleaning

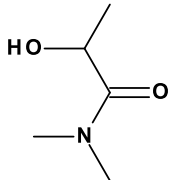
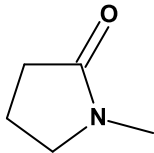

Potential Applications

- Enamel wire coatings
- Paint strippers
- Solvent for adhesives formulations
- Lube oil extraction / recycling
- Foundry
- Degreasing

Agnique® AMD 3 L

Comparison with NMP

Solvent Properties

Product	AMD 3L	NMP
CAS No.	35123-06-9	872-50-4
Formula		
Classification	NONE	
SVHC ⁽¹⁾	no	SVHC
m.p. / b.p. [°C]	-60 ⁽²⁾ / 223	-23 / 204
Flash point [°C]	103	91
Water solubility	Miscible	Miscible
Vapor pressure 20°C [hPa]	< 0.1	0.32
Viscosity 20°C [mPa*s]	5,1	1,7

⁽¹⁾ Substances of Very High Concern

⁽²⁾ Pour point

Example: Solvent Recycling

Product	AMD 3L	NMP
Recycling Yield	89% (99,1% GC purity)	85%



Mixture:

15% AMD 3L (NMP)
10% glycerol
75% water

Two-step distillation:

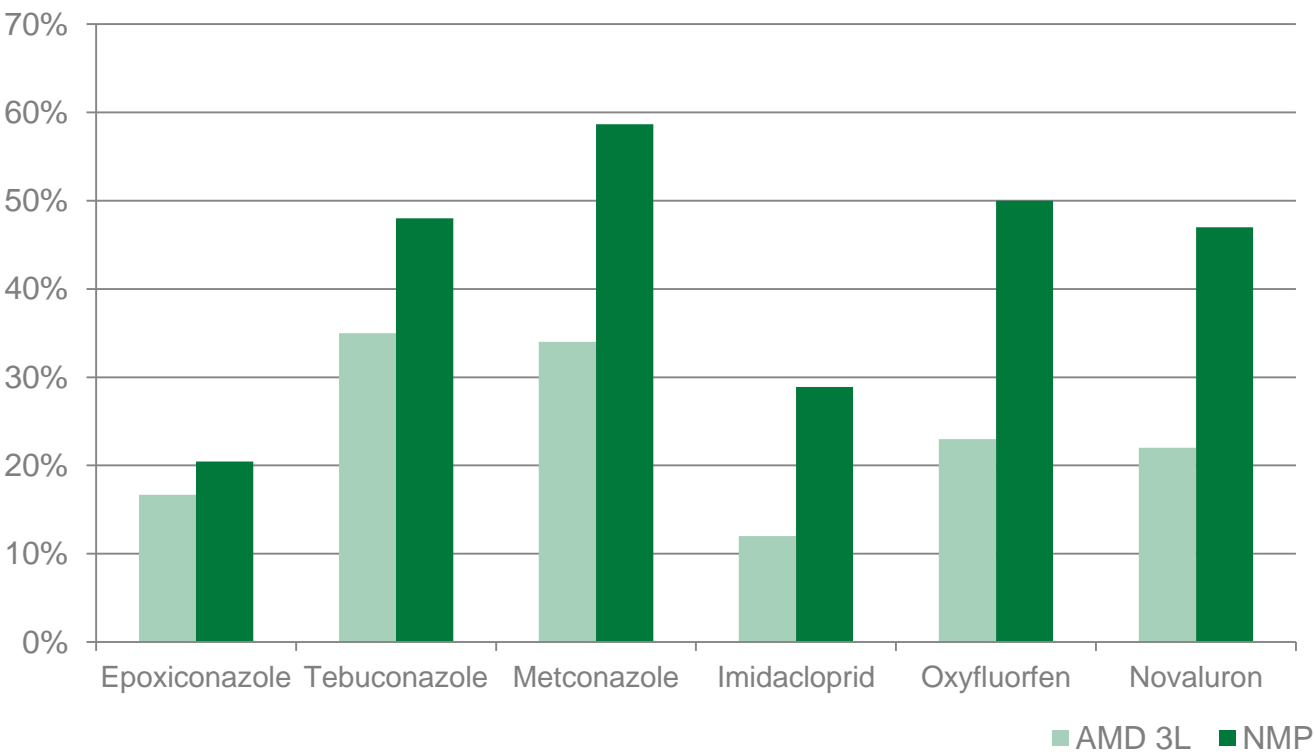
1. Water (50°C, 140 mbar)
2. AMD 3L (NMP) (60-65 mbar, 120-130°C)

Agnique® AMD 3 L

Application in Agchem Formulations

- Agnique® AMD 3 L is used as a solvent for Agchem. Formulations
- Solvency power for active ingredients is in the range of NMP

Solvency comparison with NMP:



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Dissolving of Plastics

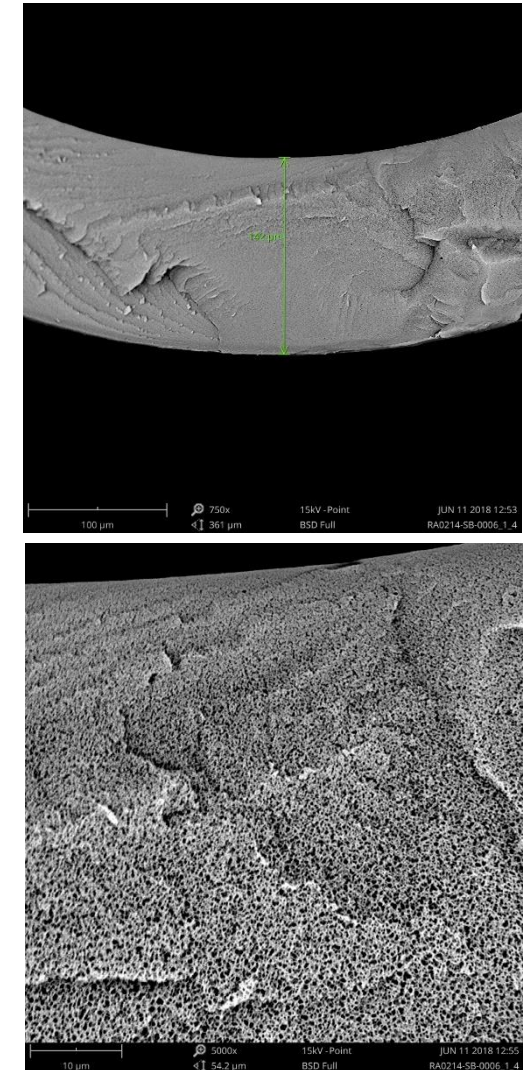
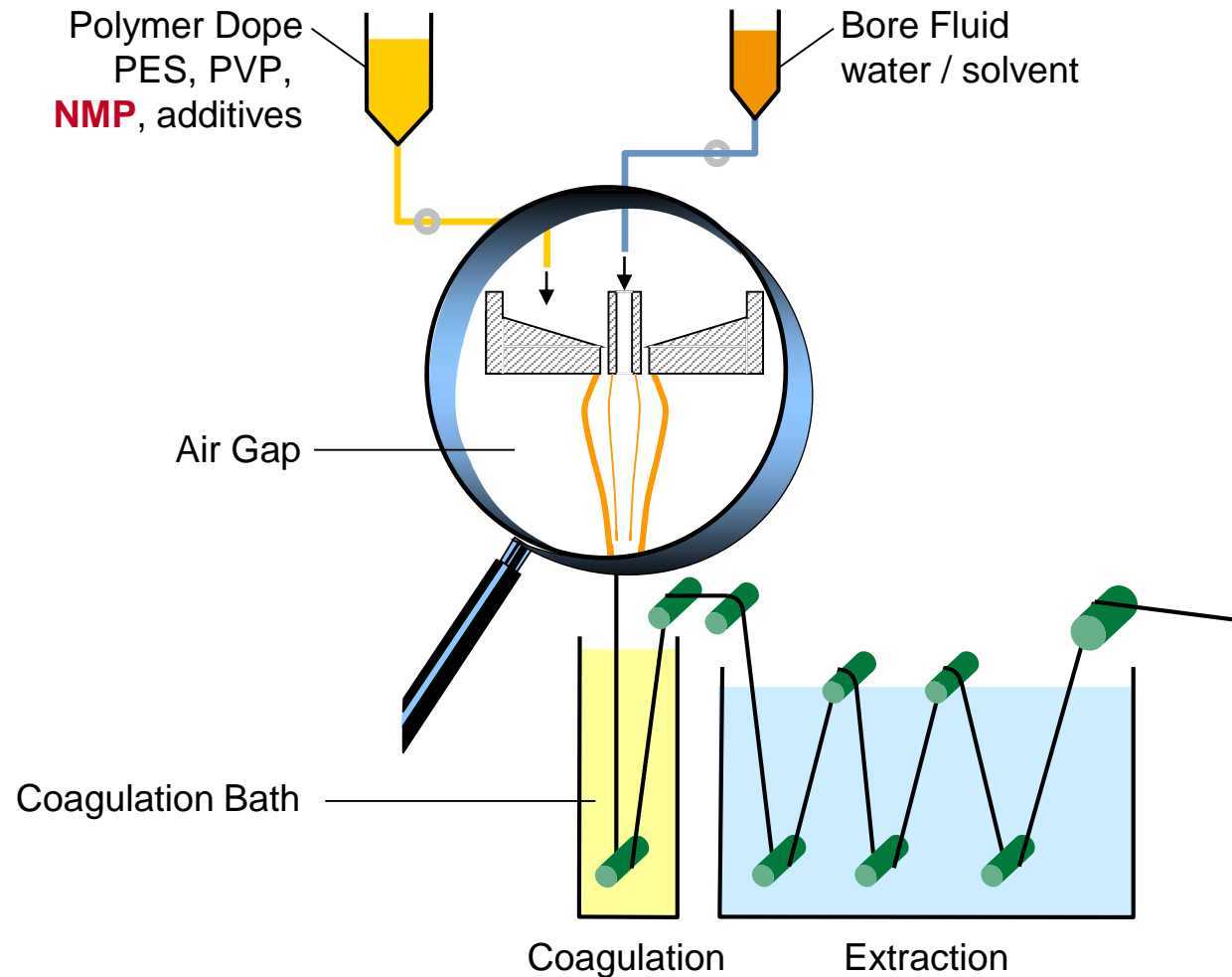
Dissolving Tests at room temperature (10% of plastic solution):

Plastic Type	Soluble
Polyethersulfone	✓
Polyurethane	✓
Polymethylmethacrylate	✓
Poly(styrene-co-acrylnitrile)	✓
Polyvinylchloride	✓
Polysulfone	✓
Polyphenylsulfone	✓
Polyamide	✗
Polyalkylterephthalate	✗
PVDF	✗



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Application for Ultrafiltration Membranes

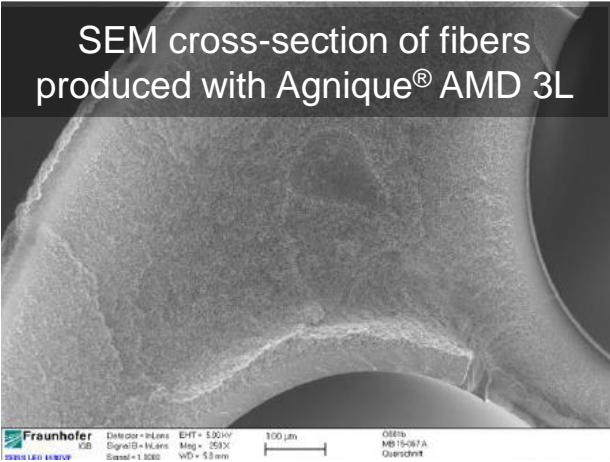
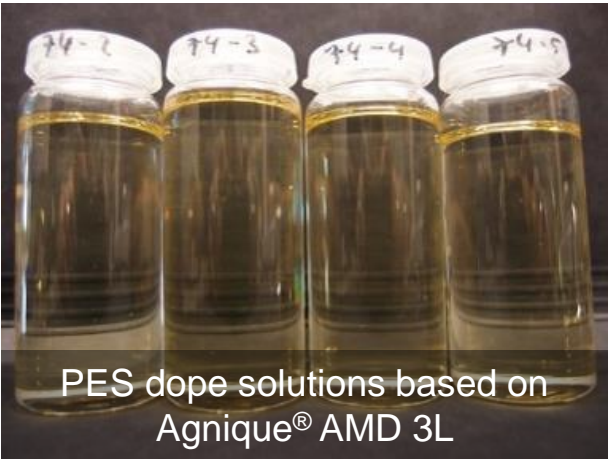


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Application for Ultrafiltration Membranes

Agnique® AMD 3L has been successfully applied to produce PES based ultrafiltration membranes

	NMP based formulation	AMD 3L based formulation
Polyethersulfone (PES)	19 wt.%	19 wt.%
Polar co-solvent	Required	Not required
Dynamic Viscosity	~ 20 Pa*s	20 - 25 Pa*s
Appearance	clear, transparent	clear, transparent



Agnique® AMD 3 L

Green solvent for PES ultrafiltration membrane preparation

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Applied Polymer
SCIENCE

AGNIQUE AMD 3L as green solvent for polyethersulfone ultrafiltration membrane preparation

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ABSTRACT: With the advent of the green chemistry concept novel, innocuous, biodegradable solvents require introduction in industrial processes. *N,N*-dimethyl lactamide (AGNIQUE AMD 3L) represents a bio-based, biodegradable, label-free polar, protic solvent. In this article, AGNIQUE AMD 3L is introduced as novel solvent for preparation of polyethersulfone (PESU) nonsolvent-induced phase separation ultrafiltration membranes using polyvinylpyrrolidone or poly(ethylene oxide) as second dope additives. Analysis of Hansen solubility parameters indicates good solvent–polymer interactions for polymer dope compositions required for PESU membrane manufacturing. Depending on the process conditions, PESU ultrafiltration membranes with hydraulic permeability values up to $610 \text{ kg m}^{-2} \times \text{bar} \times \text{h}$ and molecular weight cutoff value of 20 kDa were obtained. Scanning electron microscope of membrane cross sections reveals perfect defect-free, asymmetric morphologies. As a result, AGNIQUE AMD 3L provides a new alternative as replacement for polar, aprotic solvents employed in membrane manufacturing so far. © 2019 Wiley Periodicals, Inc. *J. Appl. Polym. Sci.* **2019**, *136*, 48419.

KEYWORDS: biodegradable; membrane; *N,N*-dimethyl lactamide; nontoxic; polyethersulfone; solvent; ultrafiltration

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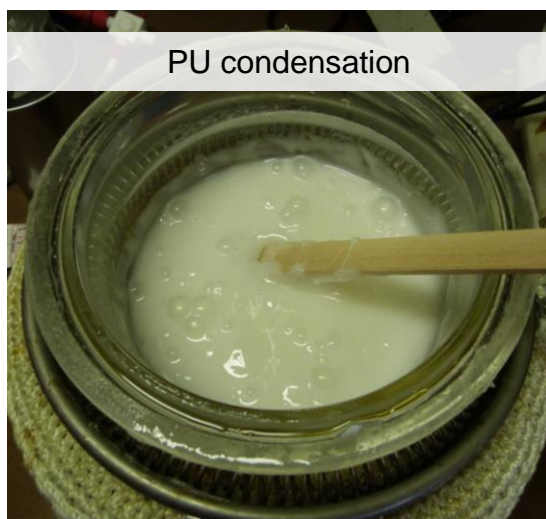
DOI: [10.1002/app.48419](https://doi.org/10.1002/app.48419)

Agnique® AMD 3 L

Solvent for polyurethane vessel cleaning

- Excellent solvency power
- Superior performance over NMP
- Polyaddition termination via hydroxy group

Example: Reactor cleaning with Agnique® AMD 3 L. Conditions: 2h at

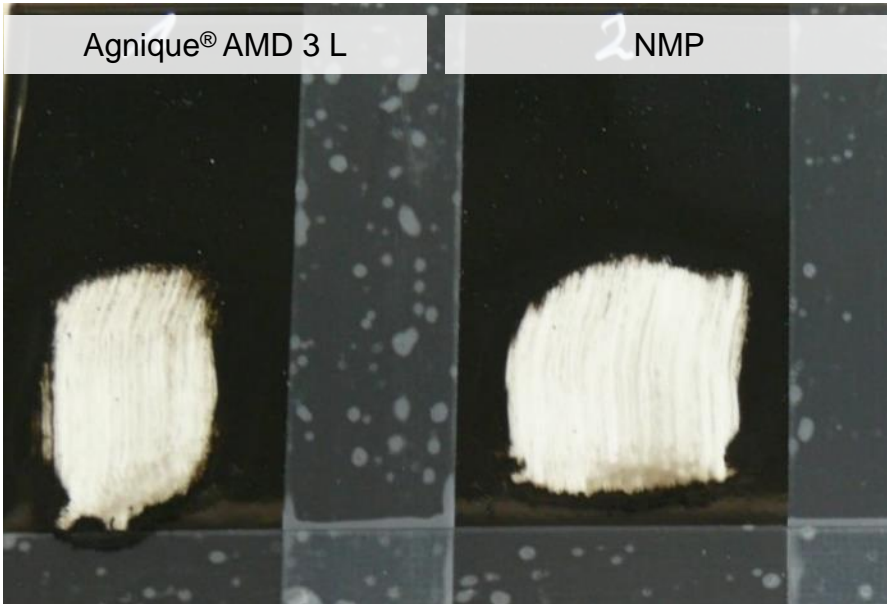


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Application for Paint Removal

Example: Removal of black graffiti from white floor tile

Conditions: Solvent (AMD 3 L or NMP) based formulation (25%) was applied on the tile for 15 min and wiped with cloth (see pictures):



Solvency power on the level of NMP



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Degreasing

Example: Degreasing of different substrates with different solvents

Substates:	Steel			Tile			Glass		
Oils:	Rape oil	White oil	Silicone oil	Rape oil	White oil	Silicone oil	Rape oil	White oil	Silicone oil
Solvent:									
Agnique® AMD 3 L	2	5	2	2	2	2	2	2	3
NMP	2	4	2	4	1	5	2	2	5
Trichloroethylene	2	1	2	2	1	1	2	1	1
Tetrachloroethylene	2	1	2	2	1	1	3	1	2

Test procedure:

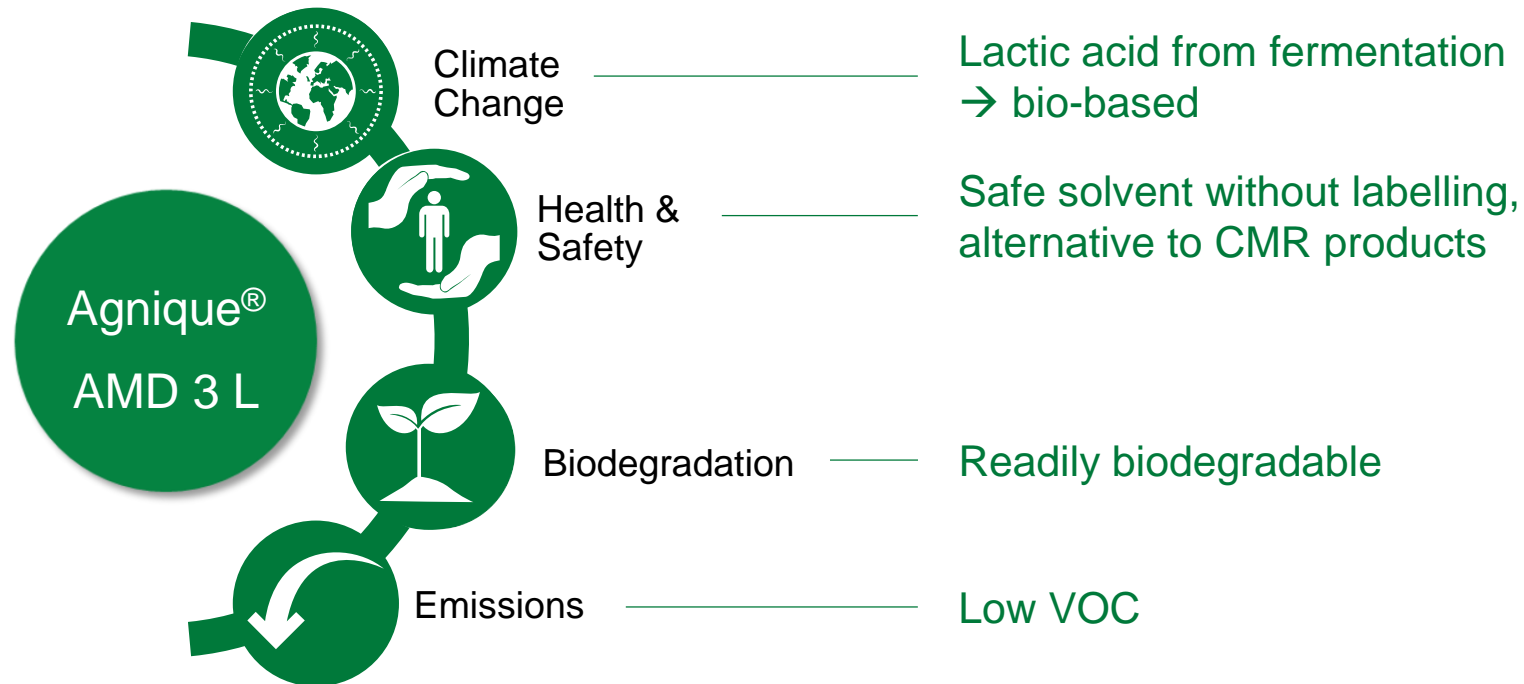
Substrates are oiled with the respective oil, dried for 24h at 60°C and another 24h at 80°C.
 Afterwards a cloth is immersed in the solvent and the surface is wiped with the soaked cloth.
 The number of wipes is documented and is an indicator for the cleaning performance.
 1 = very good; 5 = bad

Agnique® AMD 3 L shows very good degreasing performance over different types of surfaces and oils

Agnique® AMD 3 L

Sustainability Classification: Accelerator

Agnique® AMD 3L addresses four major sustainability needs of the industry and is therefore classified as **Accelerator** within the BASF Sustainable Solution Steering methodology:



Summary

- Agnique® AMD 3 L is a water-soluble sustainable solvent
- It is label-free, bio-based, readily biodegradable and REACH registered.
- Agnique® AMD 3 L offers excellent solvency power, very similar to widely used solvents like NMP or DMF, that are toxic and considered as SVHC chemicals.
- Agnique® AMD 3 L has already been applied successfully as NMP alternative in various applications.



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