

Document

# Rhodiasolv Iris, développement d'un nouveau procédé pour réduire l'empreinte environnementale des solvants

## Rhodiasolv Iris, development of new sustainable process for an improved sustainable solvent footprint

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### Résumé

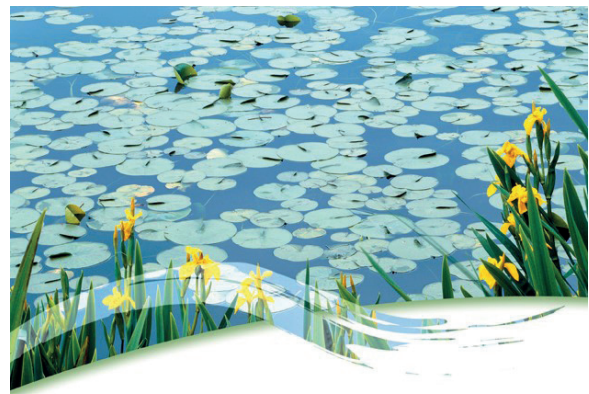
Rhodiasolv® IRIS est un solvant *diester* produit à partir d'un coproduit (MGN, 2-méthyl-glutaronitrile). Cette valorisation permet de réduire l'impact sur l'environnement (réduction de 0,5 tonne de CO<sub>2</sub> par tonne de valorisé MGN, soit une réduction globale des émissions de CO<sub>2</sub> équivalant à la libération de gaz de 16 000 voitures). Il est biodégradable, non toxique, non volatil et ininflammable, offrant ainsi des solutions efficaces et plus sûres dans divers domaines, tels que le décapage de peinture, l'enlèvement des graffitis, la dissolution de la résine ou le dégraissage industriel. L'équipe du projet du Centre de recherche et de la technologie de Lyon (*Solvay Research & Innovation Center*) a développé une chimie catalytique innovante pour transformer MGN en *diesters*. Cette chimie ne génère pas de sels et conduit à un processus énergétiquement optimisé. L'objectif du projet IRIS est de démontrer la viabilité industrielle et durable de ce nouveau procédé de fabrication de ce solvant et d'acquérir des données fiables permettant une étape directe de l'échelle pilote à l'échelle industrielle, sans investir dans une unité d'échelle intermédiaire. La fabrication de Rhodiasolv® Iris est un processus de réaction en deux étapes, avec une récupération de tous les coproduits générés.

3 phases de développement ont été suivies :

- acquisition de données de base, (cinétique, thermodynamique liquide équilibre/vapeur, solubilités...), définition des modèles de mécanismes et de tous les phénomènes observés ;
- conception et réalisation d'un projet pilote à l'échelle du laboratoire pour acquérir des données (effet de recyclage, la durée des

catalyseurs...) et de validation/ajustement des modèles ;

- ensuite, validation des modèles consolidés de simulation en exécutant un long terme (3 mois).



## Introduction

Rhodiasolv® IRIS is a diester solvent produced from a Solvay well-known co-product (MGN, 2-methyl-glutaronitrile). This valorisation enables us to optimise our non-renewable materials footprint and then reduce our environmental impact (reduction of 0.5 ton of CO<sub>2</sub> per ton of valorised MGN which may represent at maturity a global CO<sub>2</sub> reduction equivalent to the 16 000 cars' gas release).

Rhodiasolv® Iris is biodegradable, nontoxic, non-volatile and non-flammable offering then efficient and safer solutions in various fields like paint stripping, graffiti removal, resin dissolution or industrial degreasing.

To enable a sustainable and long term viable model, the project team in the Lyon Research Center and Technology (Solvay Research & Innovation Center in Lyon) developed an innovative catalytic chemistry to transform MGN into diesters. This chemistry doesn't generate any salts and leads to an energetically optimised process.

The goal of IRIS project is to demonstrate the industrial and sustainable viability of this new process to manufacture this solvent and acquire robust data enabling a direct step from pilot scale to industrial without investing an intermediate scale unit.

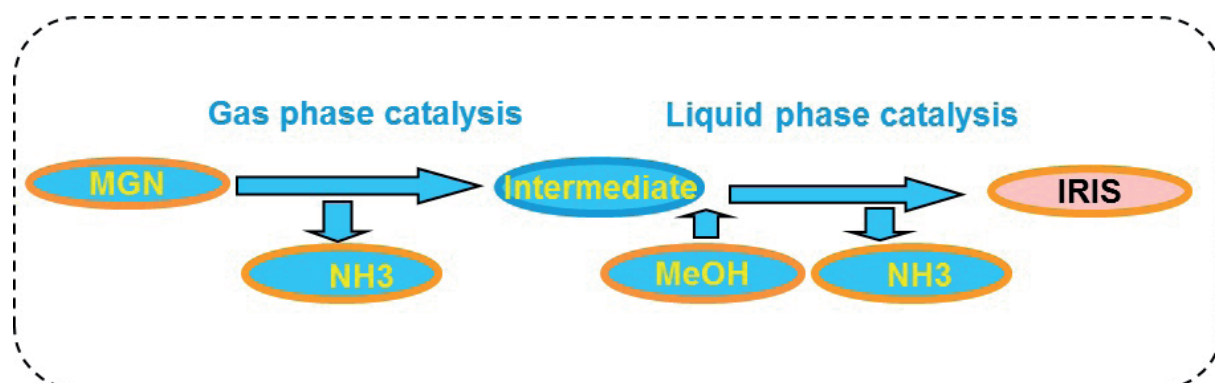
The manufacturing of Rhodiasolv® Iris is a two-step reaction process with a recovery of all co-products generated.

The project aims to develop these two chemistries and associated technologies (reactors and separation) allowing to reach the goals of the development of sustainable conditions.

The project's organisation is focused on the three main axis :

- Basic data acquisition, (kinetics, thermodynamics liquid/vapour equilibrium, solubilities...) and definition of models describing mechanisms and all the observed phenomena.
- Conception and realisation of a laboratory scale pilot to acquire data (recycling effect, catalysts duration...) and validation/adjustment of the models.
- Then, validation of the consolidated models of simulation by running a long term (3 months) run.

The technical part of this project is to get robust lab and pilot studies to build numerical models definition for scale-up and simulation. These results will also be used to assess and confirm the sustainability of this solvent manufactured via this process by revisiting its Life Cycle Analysis.



Scheme 1.  
Global Synthetic Scheme.

## 1. State of the art

### *What is the current state of the art ?*

- ✓ Solvent are often volatile and/or toxic for human and/or environment

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- ✓ Industrialisation of a high volumes product requires long development times and goes from lab to industrial unit through multi scale steps

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- ✓ Commonly used solvent don't have always a good environmental footprint as their sustainable indexes can show

### *What are we trying to achieve ?*

- Rhodiasol® Iris brings a safer solution on the market by having a low VOC, non-toxic for human and environment, biodegradable footprint

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- ✓ In the Iris project, the methodology based on software modelisation helps us to shorten development times and reduces the number of intermediate scale needed for the industrialisation

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- ✓ With the described and original process, where all streams are recycled efficiently, we are able to provide a sustainable solution to the end user by improving greatly its whole footprint.

Our approach avoiding intermediate scale-up validation can be replicated and skipping this intermediate scale validation step is an important saving of time and money in the development of new products and technologies.

## 2. The Demonstrator Phase 1

The goal of this demonstrator was to validate lab results, acquire robust and trustable data then validate at kilogram scale the whole process to get efficiently the intermediate from MGN to Rhodiasolv® Iris.

The robust acquired data will in a next step allow us to build and feed software models to simulate future industrial unit.

### **Main results**

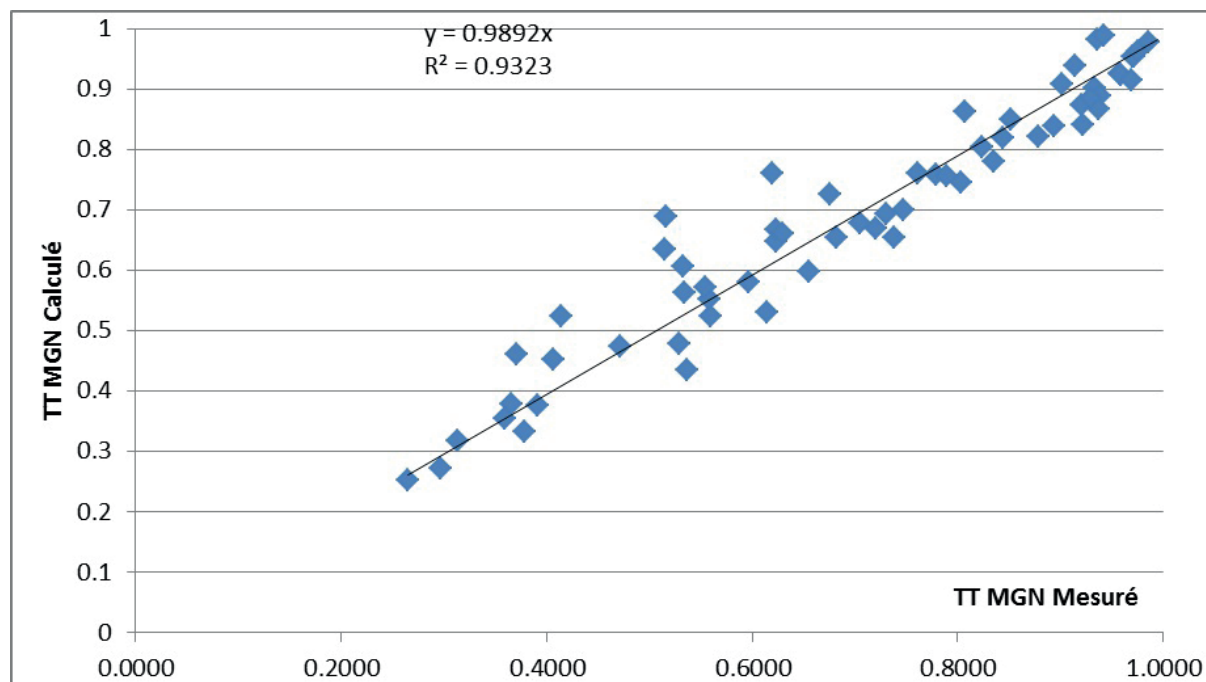
A lab screening able to transform efficiently MGN to the first intermediate to Rhodiasolv® Iris allows us to select an efficient catalyst and the best conditions to perform efficiently the required transformation. Thanks to these conditions and an efficient recovery of the co-products, we were able to produce efficiently Rhodiasolv® Iris with a great impact on sustainable indexes.

The demonstrator built allows the lab results validation, robust and trustable data acquisition then validation at kilogram scale of the whole process.



Picture 1.  
Demonstrator Gas Phase Reactor.

We were also able to build extrapolation numerical models which allow industrial conditions simulations. The following table shows the correlation between estimated MGN conversion vs. measured in the pilot.



Graph 1.

Example of correlation between calculated and experimental data.

### 3. The Demonstrator Phase 2

The goal of this demonstrator was to validate lab results, acquire robust and trustable data then validate at kilogram scale the whole process to transform efficiently the intermediate from phase 2 to Rhodiasolv® Iris.

The robust acquired data will in a next step allow us to build and feed software models to simulate future industrial unit.

#### **Main results**

A lab screening able to transform efficiently the step 1 intermediate to Rhodiasolv® Iris allow us to select a rare earth based catalyst and the best conditions fixed high pressure conditions for the reaction and ammonia recovery steps. We also evaluate a reactive distillation to prepare this product. Thanks to these uncommon conditions, we were able to produce efficiently Rhodiasolv® Iris with a great impact on sustainable indexes.

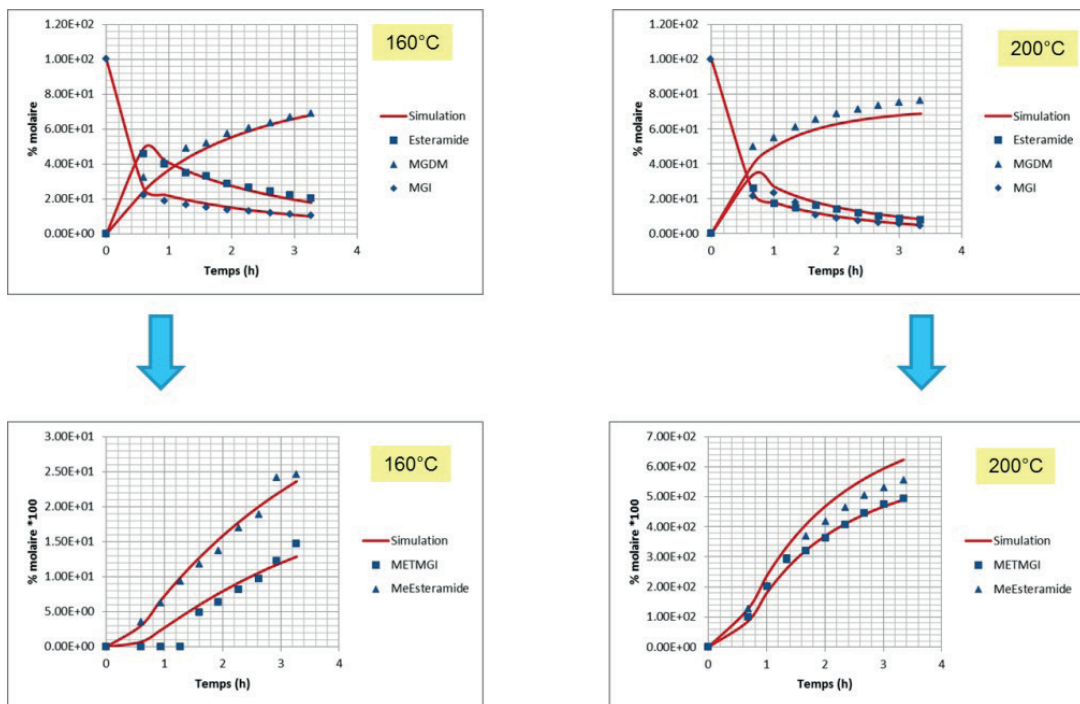
The demonstrator built allows the lab results validation, robust and trustable data acquisition then validation at kilogram scale of the whole process.



Picture 2.

Demonstrator for Distillation under Positive Pressure.

We were also able to build extrapolation numerical models which allow industrial conditions simulations. The following tables show the difference between simulation and measured concentrations of various identified intermediates formed during this step.



Graph 2.

Example of correlation between calculated and experimental data – kinetic data for step 2.

## 4. Environmental benefits

As shown by the table, Rhodiasolv® Iris is a solution bringing important benefits compared to common solvent used in the same application. It has an improved Hygiene Safety & Environment profile as it is biodegradable, not volatile and not toxic.

As no significant amount of effluent comes out of this revisited process and the yields are really good, the revisited sustainable indexes show a great improvement mainly in climate changes and resources consumption. These results confirm the initial motivations to embark in this project with the great help of Ademe & Life +.

Solvent	Flammability (Flash point)	Evaporation lose	Health and safety
<u>IRIS</u>	Non flammable	Very low	Non toxic Non irritant
Acetone	Flammable	Very high	Flammable
Methylene chloride	Non flammable	Very high	Toxic Pot. Carc.
NMP	86°C	Low	Reprotoxic

NMP : N-methyl-pyrrolidinone

Table 1.

Some key properties of commonly used solvents.

Damage Category	Rhodiasolv ® Iris New	Rhodiasolv ® Iris	Unit
	Route	Initial Route	
Climate Change	1,76	4,38	Kg CO2 eq
Resources	47	103	MJ primary
<i>Human Health</i>	$0,36 \cdot 10^{-6}$	$2,4 \cdot 10^{-6}$	<i>DALYs</i>
<i>Ecosystem Quality</i>	0,076	0,0336	<i>PDF*m<sup>2</sup>*yr</i>

*DALYs: Disability Adjusted Life Year*

*PDF x m<sup>2</sup> x yr : Potentially disappeared Fraction x m<sup>2</sup> x year*

Table 2.  
Rhodiasolv® Iris Routes Sustainable Indexes.

We would like to thank all the colleagues from the Research and Innovation Center of Lyon who participate to this project and without whom it wouldn't have been possible to transform this great idea in such a success.

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