



LUBRICANT
EXPO

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Digital AI Based Formulation Development Platform for Crankcase Lubricants

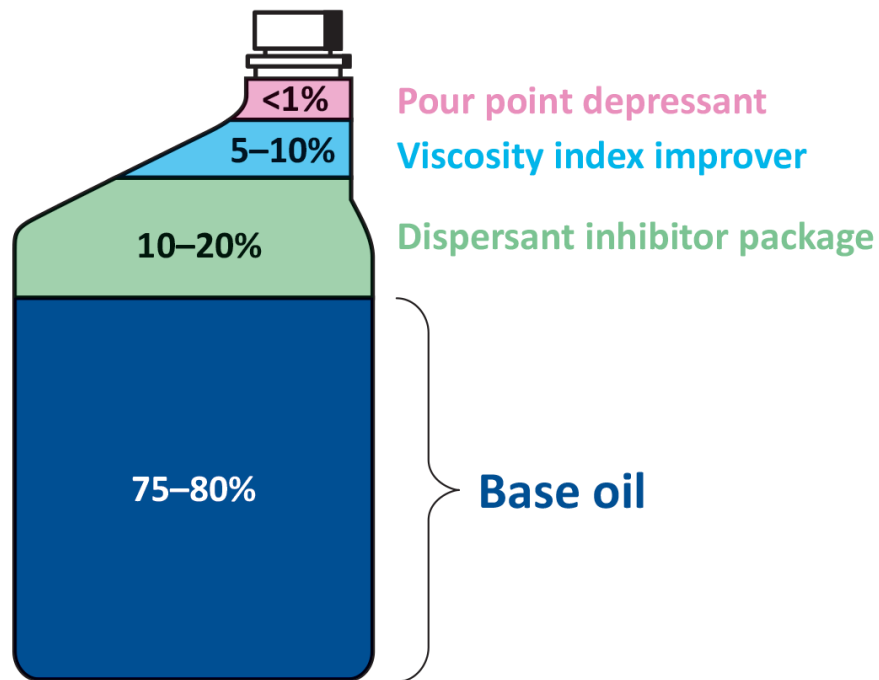
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Based on SAE Tech. Paper 2022-01-1096

Crankcase lubricant formulation



Dummy formula SAE 10W-40:

Base oil 150N	80.0
DI package	10.8
VII additive	9.2
=====	
Total	100%

The physicochemical properties

Properties of the finished product are determined by the properties of its constituents:

$$\left\{ \begin{array}{l} p_1 = F_1(p_{11}, p_{12}, p_{13}, \dots p_{1N}, x_1, x_2, \dots, x_N) \\ p_2 = F_2(p_{21}, p_{22}, p_{23}, \dots p_{2N}, x_1, x_2, \dots, x_N) \\ p_3 = F_3(p_{31}, p_{32}, p_{33}, \dots p_{3N}, x_1, x_2, \dots, x_N) \\ \\ p_M = F_M(p_{M1}, p_{M2}, p_{M3}, \dots p_{MN}, x_1, x_2, \dots, x_N) \end{array} \right.$$

P_i ($i = 1, \dots, M$) is the i th property of the blend

p_{ij} is the i th property of the j th component of the blend

$x_j (j=1, \dots, N)$ is the weight fraction of the j th component

F_i is the corresponding functional property-blending relationship

Which properties

Raw materials:

Physical

(KV100, KV40, etc.)

Chemical

(PAO, ester, Ca, S, P, ...)

Commercial

(Price, MOQ, ...)

etc

Finished product:

Physical

(KV100, KV40, CCS, HTHS, Noack, Elastomer...)

Chemical

(P, S, SA)

Engine tests

(Sequence VID, VIII, IIIG,)

Commercial

(Price, ...)

etc

Property-composition relationships

Sparse and noisy data

Base oil:

KV100, KV40, Noack,
Seal compatibility, Density,
FP, PP, HTHS, CCS

DI package:

KV100, KV40, TBN,
Oxidation stability, Engine
test Sequences outcome

PPD additive:

PP, CCS

VI improver:

KV100, KV40, HTHS, CCS

Bayesian optimization is very useful when working with complex and noisy functions

Example: Viscosity blending

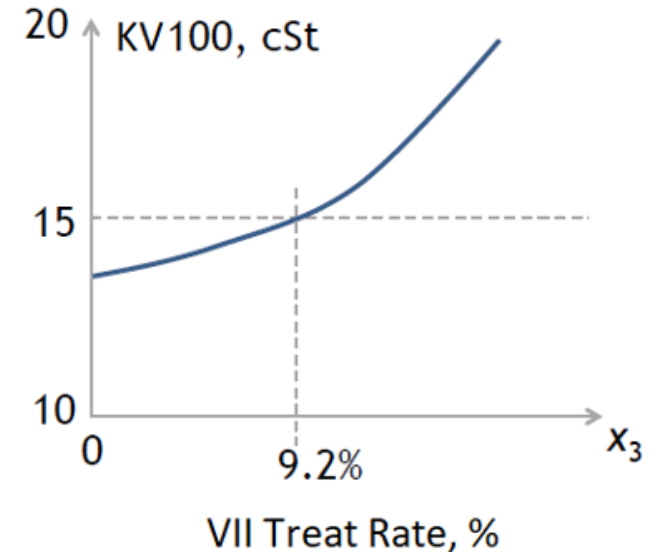
Let's assume we want to formulate a SAE 10W-40 oil with KV100 = 15 cSt from the following raw materials:

1. Base oil: KV100 = 6 cSt80.0%
2. DI package: KV100 = 240 cSt10.8%
3. VI improver: KV100 = 1000 cSt9.2%

DI treat rate is specified by the manufacturer at 10.8%.

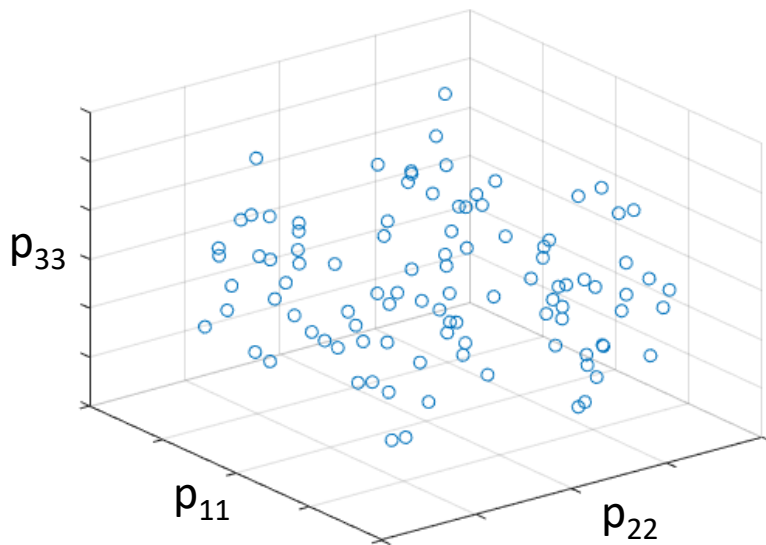
Futhermore, $x_1 + x_2 + x_3 = 100\%$

Hence: KV100 of the product is a function of x_3 only:

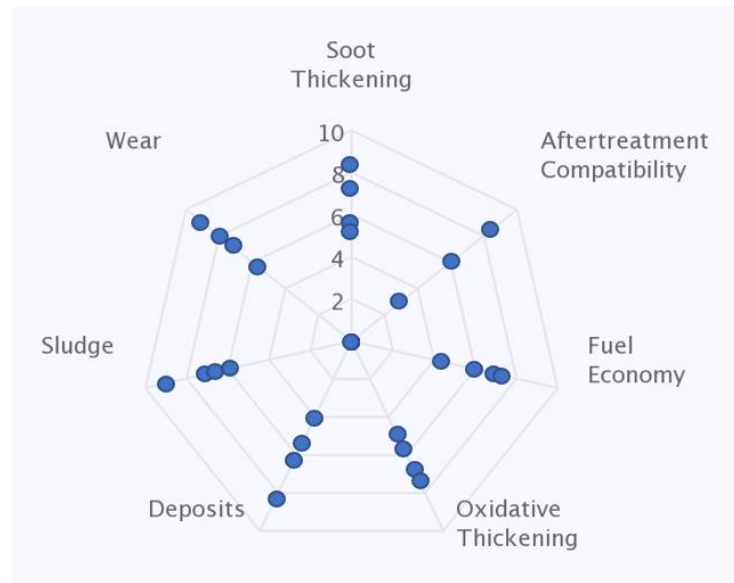


Generalized property mapping

Properties of raw materials

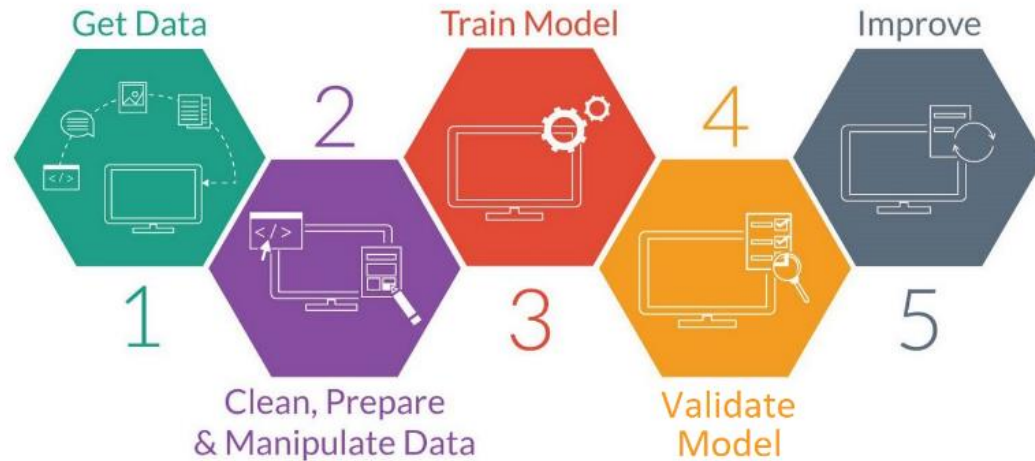


Properties of finished product

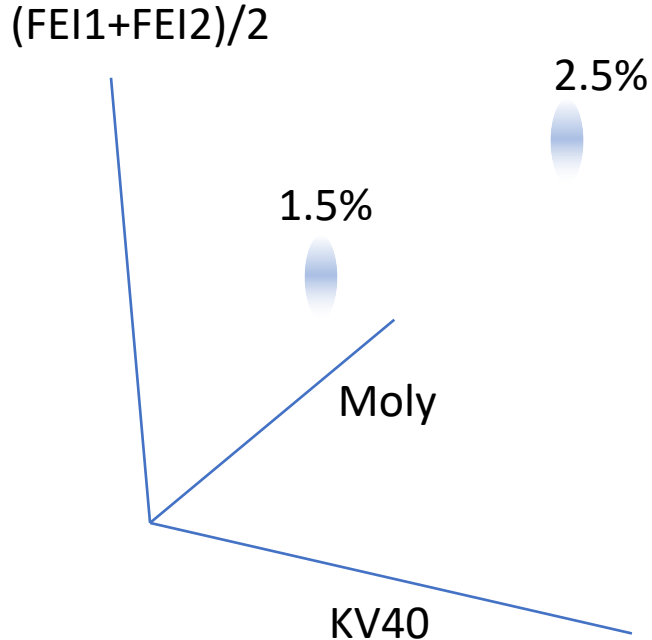


A generalized property space may have 10 to 30 dimensions!

Reconstructing property-composition relationships using AI / ML approach



Handling scarce data: Homologation tests



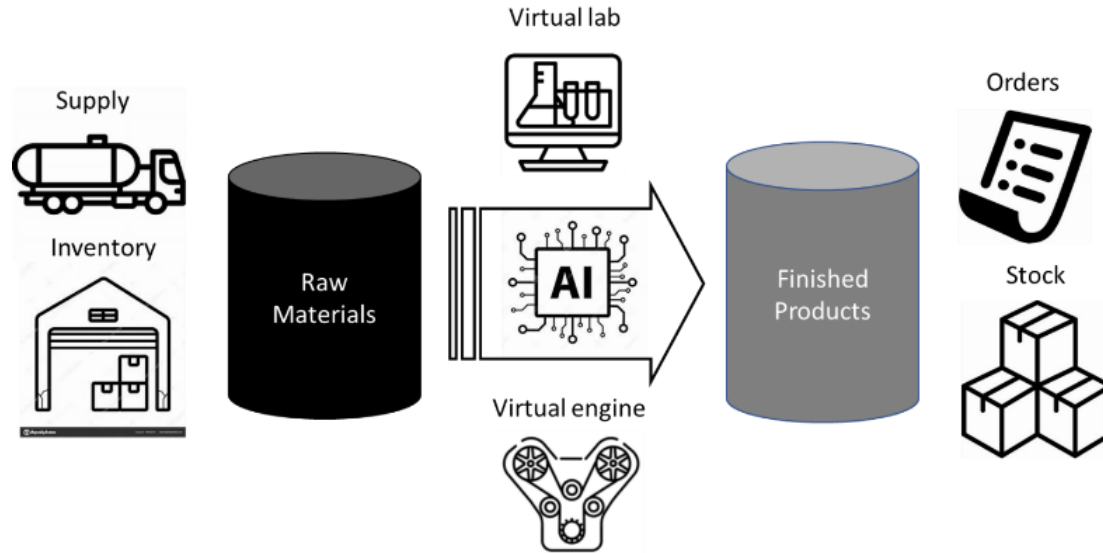
Let's assume you have carried out Sequence VI F (ASTM D8226) data for 2 SAE 0W-16 motor oil formulas with identical HTHS but different KV40 and molybdenum content.

Two points in the middle of nowhere. Mind the test uncertainty, $\sim 0.2\%$.

Not very useful.

What if you have a “virtual” 3.6L GM engine?

Two measured points can be used to calibrate the model.



One can perform virtual Sequence VI (GM V6 PFI), CEC L-54-96 (M111) and JASO FE M366 (Toyota 2ZR-FXE) tests to address both API/ILSAC and ACEA requirements.

Example: Cost optimization

PCMO SAE 5W-30 ACEA C3

Original formula

Ingredient	Percentage	Price, € / kg	Historical MOQ and quantity to order
Base oil 1, API Gr. IV	10	3.0	1 IBC (1000L, 820kg) => 3 IBCs/20 t
Base oil 2, API Gr. III	40	1.5	1 IBC (1000L, 830kg) => 10 IBCs/20t
Base oil 3, API Gr. II	30	1.0	1 IBC (1000L, 860kg) => 7 IBCs/20t
VI improver (OCP)	8	1.5	1 drum (200L, 174kg) => 10 drums/20t
VII / PPD (PAMA)	2	5.0	1 drum (200L, 186kg) => 3 drums/20t
Add-pack	10	4.5	1 IBC (1000L, 870kg) => 3 IBCs/20t
Total	100%	<u>Raw material cost:</u> 1.87 € / kg theoretical (without material excesses) 2.15 € / kg actual (with material excesses)	

Optimized formula

Ingredient	Percentage	Price, € / kg	Historical MOQ and quantity to order
Base oil 1, API Gr. IV	8.2	3.0	1 IBC (1000L, 820kg) => 2 IBCs/20 t
Base oil 2, API Gr. III	41.5	1.5	1 IBC (1000L, 830kg) => 10 IBCs/20t
Base oil 3, API Gr. II	29.6	1.0	1 IBC (1000L, 860kg) => 7 IBCs/20t
VI improver (OCP)	8.9	1.5	1 drum (200L, 174kg) => 10 drums/20t
VII / PPD (PAMA)	1.8	5.0	1 drum (200L, 186kg) => 2 drums/20t
Add-pack	10.0	4.5	1 IBC (1000L, 870kg) => 3 IBCs/20t
Total	100%	<u>Raw material cost:</u> 1.84 € / kg theoretical (without material excesses) 1.98 € / kg actual (with material excesses)	

Constraints: Batch size, MOQ, product specifications

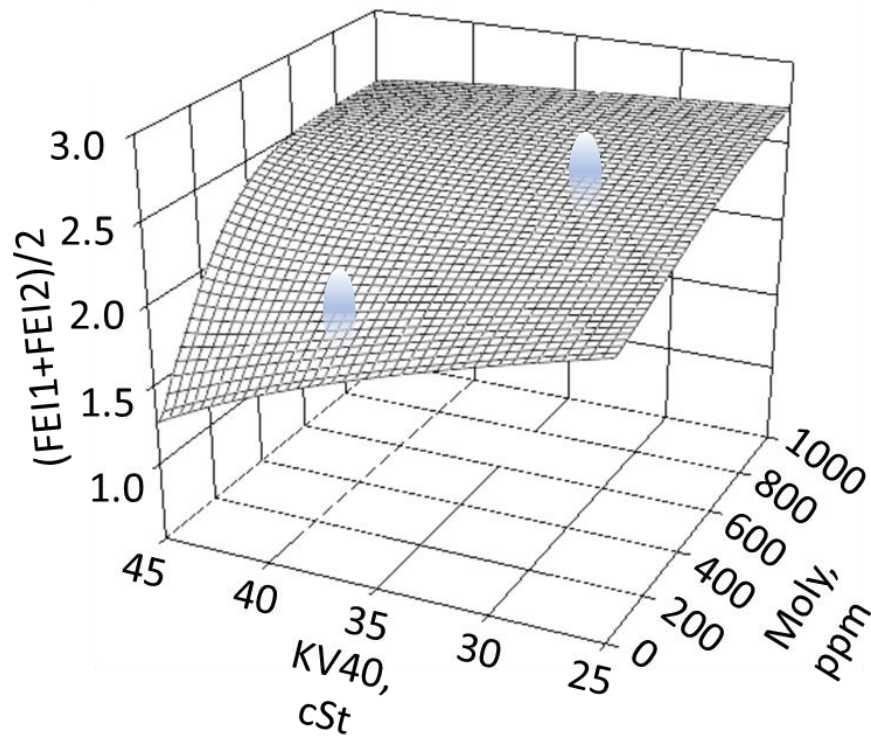
Optimization: Excess minimization

Properties comparison: all within specs

Property	PCMO SAE 5W-30 ACEA C3	
	Historical formulation	Price-optimized formulation
Kin. Visc. @ 100°C, cSt	11.5	11.6
Kin. Visc. @ 40°C, cSt	68.1	67.1
VI	165	170
CCS -30C, cP	5700	6000
Pour point, °C	-45	-42
Flash point, °C	240	240
Noack, %	9.5	9.5
TBN, mgKOH/g	7.0	7.0
SA, %	0.76	0.76

0.17 €/kg saving

Reconstructed property-composition relationship



Conclusions

- Possible applications of AI/ML tools in the lubricant industry include add-pack development and product portfolio management
- AI tools are continuously “recalibrating” themselves based on new data, including failed tests, thus constantly improving their predictive power
- The AI Formulator Assistant platform we are developing helps to speed up new formulation development and reduce associated costs
- Integration of a Virtual Engine module into the platform is expected to enable accurate predictions of homologation engine tests where available test data are scarce
- Multiple cross-correlations between different performance specifications can be exploited

Thank You!



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