Tipps&Tricks with G[raf]Compounder

No. XII
Standard Procedure for Managing Multi-Polymer Blends in GrafCompounder

Historic compound databases typically contain a broad diversity of raw materials, particularly polymers. In industrial rubber manufacturing (e.g., tire components, technical articles, vibration parts, hoses, seals), formulations generally contain a single base polymer, occasionally a binary blend, and only in exceptional cases a ternary polymer system. The use of polymer blends can, however, provide measurable technological, economic, and performance-related benefits.

AI-based compound-prediction software does not inherently recognize practical limitations related to the number or type of polymers used in one formulation. Each polymer is handled as an independent ingredient, without awareness of real-world manufacturing constraints. Consequently, when only performance targets are specified, the software may select several similar polymers (e.g., multiple natural rubbers or SBR grades) in order to mathematically satisfy target properties — even if this result is impractical or uneconomical for production.

To address this limitation in **GrafCompounder**, the following four-step procedure is recommended.

Step 1:
Initial Prediction Using Automatic Mixing

Run the **Automatic Mixing** function using the original (unfiltered) dataset. Define the desired target properties in the **Criteria** window only.

Example dataset (Table 1):

- 3 Natural Rubbers (NR)
- 6 Styrene-Butadiene Rubbers (SBR, different types)
- 1 Butadiene Rubber (BR)
- 1 Recycled Rubber
- 3 different process oils
- Various standard compounding ingredients (carbon black, curatives, etc.)

Because no explicit constraints on polymer type or number are defined, while propeerties targeted only, the AI may select several similar ingredients

Name	Min	Max
SMR 10	*0*	*100*
SMR CV60	*0*	*100*
SMR L	*0*	*100*
SBR 1500	*0*	*100*
SBR 1618	*0*	*155*
SBR 1711	*0*	*100*
SBR 1707	*0*	*137.5*
SBR 1808	*0*	*223.5*
SBR 1843	*0*	*140*
Buna CB 10	*0*	*20*
Recycled Tread	*0*	*90*

***Table 1**: Polymers used in demonstration file.*

Criteria:

Name	Min	Max	From	To	Weight	Trdoff	Output:
							Mixture1
SMR 10	*0*	*100*					23.75
SMR CV60	*0*	*100*					13
SMR L	*0*	*100*					41.5
SBR 1500	*0*	*100*					1
SBR 1618	*0*	*155*					32.1625
SBR 1711	*0*	*100*					0
SBR 1707	*0*	*137.5*					0
SBR 1808	*0*	*223.5*					0
SBR 1843	*0*	*140*					0
Buna CB 10	*0*	*20*					0
Recycled Tread	*0*	*90*					0
N 220	*0*	*60*					0
N330	*0*	*80*					2.575
N336	*0*	*40*					8.5
N550	*0*	*60*					2.575
N660	*0*	*25*					0
N762	*0*	*85*					13.2625
Ground Rubber	*0*	*20*					0
CaCO3	*0*	*20*					0
Clay	*0*	*100*					0
Silitin N	*0*	*50*					7.2625
Paraffinic Oil	*0*	*10*					0.395
Naphtenic Oil	*0*	*45*					0.2025
Aromatic Oil	*0*	*25*					0.06
ZnO	*0*	*10*					5.85
Zn-2EH	*0*	*2*					0.415
Stearic Acid	*0*	*3*					0.9525
Benzoic Acid	*0*	*0.5*					0
Paraffin Wax	*0*	*5*					0.125
Koresin	*0*	*5*					0.415
Cumar Resin	*0*	*9*					0.83

***Table 2:** Ingredients of first prediction (Initial Automatic Mixing) with properties targets only*

to optimize the objective (fitness-) function. For example, the predicted formulation may contain three different NRs and two different SBRs (see **Table 2**). While numerically valid, such a combination is generally impractical for laboratory or industrial application.

Step 2: Manual Consolidation of Polymers and Minor Ingredients

This step is performed manually by the user.

1. Transfer the predicted formulation from the **Output** window to the **Input** window using the command **“Append mixture into Input window.”**
2. In the Input window:
    - Consolidate ingredients below a selected threshold (e.g., < 1 phr or < 2 phr).
    - Merge similar polymers and oils wherever technically reasonable (e.g., combine multiple NR types into one representative NR).
    - Remove non-critical or redundant ingredients.
3. The total phr will be automatically recalculated by the software.
4. **Important:** Property values remain unchanged at this stage because no verification experiment has yet been conducted (**Table 3**).

   In the Output window, the original prediction appears as **“Mixture1.”**
   In the Input window, the simplified version appears as **“Mixture1_gc_unconfirmed.”**

Step 3: Reuse Criteria and Introduce the Reworked Formula

Copy the manually adjusted formulation (**Mixture1_gc_unconfirmed**) into the **Criteria** window, placing it in both the **“From”** and **“To”** columns **without modification.**

All previously defined property targets remain unchanged.

This step forces the software to treat the reworked formulation as an additional constraint, ensuring that the next prediction respects both:

- The original performance targets **and**
- The simplified and consolidated ingredient structure.

Step 4: New Prediction Using “Auto Mix New Mixture”

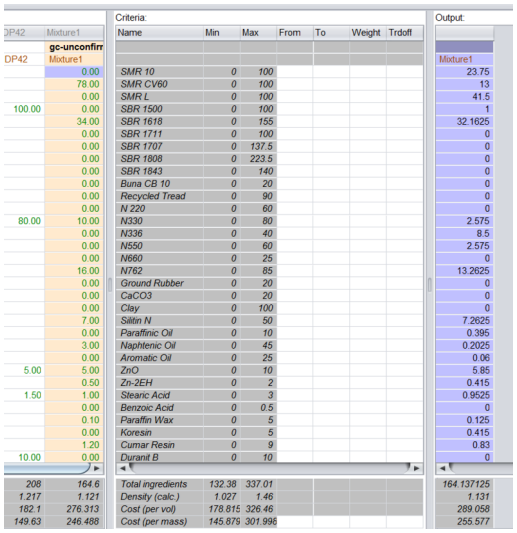

Table 3: *Reworked formula in Input window predicted compound “Mixture1” using transfer "append mixture column to input recipes." Any property is left unchanged*

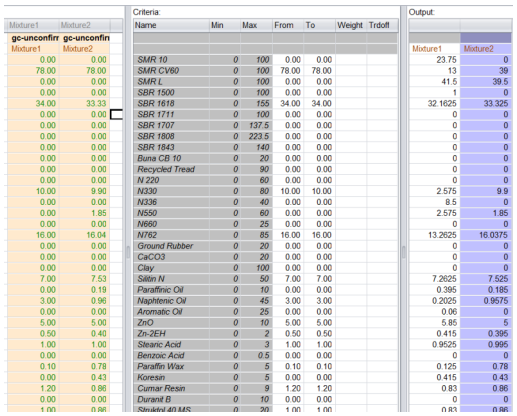

Table 4: *Transfer of adjusted formula from output window into the criteria window columns. Predict compound with “Automix New mixture”. Close procedure with “append mixure2 to input window,” select one natural rubber type , before providing formula ot the laboratory for confirmation experiment.*

Execute the function **“Auto Mix New Mixture.”**

The newly calculated compound appears in the next available column in the Output window, automatically named **“Mixture2” (Table 4)** Because both formulation architecture and performance data are used as constraints, the number of mathematical conditions increases significantly, which may result in **longer calculation times.**

In most cases, **Mixture2** will contain:

- A reduced number of polymers (e.g., one NR + one SBR instead of multiple variations)
- A more practical oil and filler system
- Property values that still meet the defined targets

For final evaluation, append **Mixture2** to the Output window and compare it directly to **Mixture1** (see **Table 5**).

Recommendation

It is **strongly recommended** to carry out confirmation experiments on **both Mixture1 and Mixture2** in order to:

- Validate the accuracy of the AI prediction
- Quantify the effect of polymer consolidation
- Confirm processability and physical properties in real laboratory conditions

Summary of the Procedure

1. Predict compound using property targets only.
2. Transfer prediction to the Input window and manually simplify the formulation.
3. Reapply both the reworked formulation and original property targets as constraints.
4. Generate a new optimized mixture for validation and final selection.

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02 December 2025
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	Recipes:	
Ingredients:	Mixture1	Mixture2
SMR 10	23.75	
SMR CV60	13.00	78.00
SMR L	41.50	
SBR 1500	1.00	
SBR 1618 (5Oil/50CB)	32.16	33.00
N330	2.58	10.00
N336	8.50	
N550	2.58	
N762	13.26	16.00
Silitin N	7.26	7.00
Paraffinic Oil	0.40	
Naphtenic Oil	0.20	2.50
Aromatic Oil	0.06	
ZnO	5.85	5.00
Zn-2EH	0.42	
Stearic Acid	0.95	1.50
Paraffin Wax	0.13	1.00
Koresin	0.42	2.50
Cumar Resin	0.83	
Struktol 40 MS	0.83	
TMQ	1.09	1.00
IPPD	2.59	2.50
PBN	0.62	
S-80	1.38	1.90
TMTD-80	0.86	0.60
CBS-80	1.93	1.60

Table 5: *After further adjustments of pocess aids with similar effects the compound has now 15 ingredients, which may be reduced even further. Finally the values should be rounded to zero or one decimal.*