

Synthesis, Production, and Mass Balance Analysis of Ten High-Volume Herbicides

Ashok K. Rathoure^{1,*}, Anika Rathoure²

Abstract

Herbicides play a crucial role in modern agriculture, enabling effective weed management and safeguarding crop yields amid rising global food demands and growing weed resistance, which can reduce productivity by up to 40%. This study provides a detailed examination of synthesis pathways, production methodologies, and mass balance dynamics for ten high-volume herbicides: Aclonifen, Ametryn, Amidosulfuron, Aminocyclopyrachlor, Aminopyralid, Atrazine, Azimsulfuron, Beflubutamid, Bensulfuron Methyl, and Bentazone, used to control broadleaf weeds, grasses, and invasives across various cropping systems. Based on stoichiometric principles and industrial data, the analysis maps multi-step chemical transformations, raw material inputs, solvent usage, byproduct generation, and waste streams at a one-ton production scale. Manufacturing sequences vary in complexity: Aclonifen synthesis involves nitration, amination, and phenylation, producing trichlorobenzene, phenol, and HCl byproducts; Atrazine's two-step amination yields NaCl and organic residues; other herbicides generate HCl, NaCl, or phenol as primary byproducts. Solvents, including toluene and ethanol (up to 3,200 kg), are largely recovered (95–98%), while neutralization requires NaOH (325–849 kg) and effluent management through ETP, TSDF, or incineration. Water inputs (1,500–8,000 kg) contribute significantly to effluent volumes. Total production footprints range from 5,811 to 15,287 kg/t, with solvent losses of 1–5% and organic losses of 2–20%. These mass balances highlight environmental challenges, including hazardous emissions, and underscore the importance of process improvements such as catalytic optimization, closed-loop solvent recovery, and bio-based alternatives. By offering granular data for lifecycle assessment, the study supports sustainable herbicide manufacturing, regulatory compliance, and innovation in agrochemical production.

Keywords: Herbicides, chemical synthesis, mass balance, byproducts, solvents, waste management

INTRODUCTION

Herbicides are indispensable in modern agriculture, providing effective weed control to maximize crop productivity and ensure food security [1–3]. The global demand for herbicides has surged due to increasing agricultural intensification and the need to combat weed resistance, which can reduce crop yields by up to 40% if not managed effectively [3–5]. The production of herbicides involves intricate

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chemical synthesis processes, requiring meticulous management of raw materials, solvents, and byproducts to optimize efficiency and minimize environmental impact [5–10]. This study examines the synthesis pathways, production methods, and mass balances of 10 high-volume herbicides, each identified by its Chemical Abstracts Service (CAS) number, as listed in Table 1. These herbicides are widely used across various agricultural systems due to their efficacy in targeting broadleaf weeds, grasses, and other invasive species [6, 7, 11]. The analysis details the chemical reactions involved, including stoichiometry, to account for all inputs and outputs, such as reactants, products,

byproducts, and waste streams [10–12]. By employing a mass balance approach, this study quantifies resource utilization and waste generation, providing a foundation for improving production efficiency and sustainability. The environmental implications of herbicide production, including the generation of hazardous byproducts like hydrochloric acid and phenol, underscore the need for advanced waste management strategies to comply with regulatory frameworks. This work aims to support the agrochemical industry in optimizing processes, reducing environmental footprints, and ensuring compliance with global regulations, such as those outlined by the United States Environmental Protection Agency [6, 11, 12].

Table 1. List of herbicides analyzed with CAS numbers.

Herbicide	CAS number	End uses
Aclonifen	74070-46-5	Pre-emergence control of broadleaf and grass weeds in cereals (wheat, barley), potatoes, sunflowers, carrots, peas, and other vegetables.
Ametryn	834-12-8	Control of broadleaf and grassy weeds in sugarcane, pineapple, bananas, corn, potatoes, and sweet corn.
Amidosulfuron	120923-37-7	Post-emergence control of annual broadleaf weeds (e.g., cleavers, docks) in cereals (wheat, barley, oats, rye, triticale), flax, linseed, and grassland.
Aminocyclopyrachlor	858956-08-8	Pre- and post-emergent control of broadleaf weeds in non-crop areas, including rangeland, pastures, rights-of-way, turf, forestry site preparation, and wildlife management areas.
Aminopyralid	150114-71-9	Control of broadleaf weeds and woody brush in pastures, rangeland, wheat, corn, hayfields, and non-crop areas.
Atrazine	1912-24-9	Pre- and post-emergence control of broadleaf and grassy weeds in corn, sorghum, sugarcane, wheat, and turf.
Azimsulfuron	120162-55-2	Post-emergence control of broadleaf weeds, sedges, and barnyard grass in rice (paddy fields).
Beflubutamid	113614-08-7	Pre- and early post-emergence control of broadleaf weeds in cereals (wheat, barley, rye, triticale).
Bensulfuron Methyl	83055-99-6	Post-emergence control of broadleaf and sedge weeds in rice and spring cereals (wheat, barley, oats, rye, triticale).
Bentazone	25057-89-0	Post-emergence control of broadleaf weeds and sedges in soybeans, rice, corn, beans, peas, sorghum, peanuts, alfalfa, and turf.

ACLONIFEN CAS# 74070-46-5

Manufacturing Process

Step 1: 1,2,3-trichlorobenzene reacts with nitric acid to form 1,2,3-trichloro-4-nitrobenzene.

Step 2: 1,2,3-trichloro-4-nitrobenzene reacts with ammonia to form 2,3-dichloro-6-nitroaniline.

Step 3: 2,3-dichloro-6-nitroaniline reacts with phenol to form Aclonifen.

Basic Chemistry

Step 1: 1,2,3-trichlorobenzene (MF: C₆H₃Cl₃ MW: 181.4 g/mol) reacts with nitric acid (MF: HNO₃ MW: 63.013 g/mol) to form 1,2,3-trichloro-4-nitrobenzene (MF: C₆H₂Cl₃NO₂ MW: 226.4 g/mol) (Figure 1).

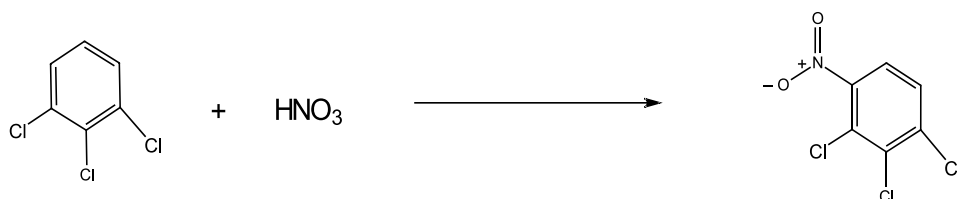


Figure 1. 1,2,3-trichlorobenzene reacts with nitric acid to form 1,2,3-trichloro-4-nitrobenzene.

Step 2: 1,2,3-trichloro-4-nitrobenzene (MF: C₆H₂Cl₃NO₂ MW: 226.4 g/mol) reacts with ammonia (MF: H₃N MW: 17.031 g/mol) to form 2,3-dichloro-6-nitroaniline (MF: C₆H₄Cl₂N₂O₂ MW:

207.01 g/mol) (Figure 2).

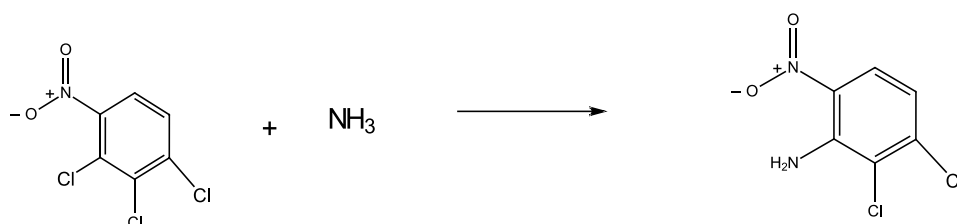


Figure 2. 1,2,3-trichloro-4-nitrobenzene reacts with ammonia to form 2,3-dichloro-6-nitroaniline.

Step 3: 2,3-dichloro-6-nitroaniline (MF: C₆H₄Cl₂N₂O₂ MW: 207.01 g/mol) reacts with phenol (MF: C₆H₆O MW: 94.11 g/mol) to form Aclonifen (MF: C₁₂H₉ClN₂O₃ MW: 264.66 g/mol) (Figure 3).

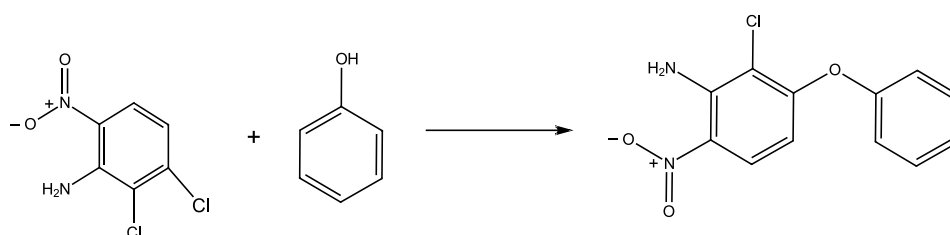
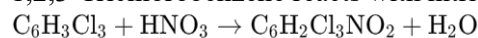


Figure 3. 2,3-dichloro-6-nitroaniline reacts with phenol to form aclonifen.

Step 1: Nitration of 1,2,3-trichlorobenzene

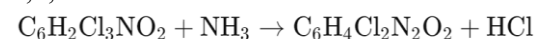
1,2,3-Trichlorobenzene reacts with nitric acid to form 1,2,3-trichloro-4-nitrobenzene.



- 1,2,3-Trichlorobenzene (C₆H₃Cl₃): MW=181.4 g/mol
- Nitric Acid (HNO₃): MW=63.01 g/mol
- 1,2,3-Trichloro-4-nitrobenzene (C₆H₂Cl₃NO₂): MW=226.4 g/mol
- Water (H₂O): MW=18.015 g/mol

Step 2: Amination of 1,2,3-trichloro-4-nitrobenzene

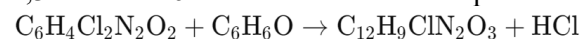
1,2,3-Trichloro-4-nitrobenzene reacts with ammonia to form 2,3-dichloro-6-nitroaniline.



- 1,2,3-Trichloro-4-nitrobenzene (C₆H₂Cl₃NO₂): MW=226.4 g/mol
- Ammonia (NH₃): MW=17.03 g/mol
- 2,3-Dichloro-6-nitroaniline (C₆H₄Cl₂N₂O₂): MW=207.01 g/mol
- Hydrogen chloride (HCl): MW=36.46 g/mol

Step 3: Reaction with Phenol

2,3-Dichloro-6-nitroaniline reacts with phenol to form Aclonifen.



- 2,3-Dichloro-6-nitroaniline (C₆H₄Cl₂N₂O₂): MW=207.01 g/mol
- Phenol (C₆H₆O): MW=94.11 g/mol
- Aclonifen (C₁₂H₉ClN₂O₃): MW=264.66 g/mol
- Hydrogen chloride (HCl): MW=36.46 g/mol

Byproducts

1. *Step 1:* H₂O: Produced during nitration.
2. *Step 2:* HCl: Produced during the amination. For every mole of 1,2,3-trichloro-4-nitrobenzene, 1 mole of HCl is produced.
3. *Step 3:* HCl: Produced during the reaction with phenol. For every mole of 2,3-dichloro-6-

nitroaniline, 1 mole of HCl is produced.

Solvent Required: Toluene or Ethyl Acetate: Approximately 1.2 to 2 times the weight of the reactants.

Calculation of Mass Balance

MW of Aclonifen: 264.66 g/mol

Moles of Aclonifen in 1 t:

$$\frac{1000 \text{ kg}}{264.66 \text{ g/mol}} = 3,779.6 \text{ moles}$$

Step-Wise Reactant Quantities

Step 1 (1,2,3-Trichlorobenzene to 1,2,3-Trichloro-4-nitrobenzene):

- Moles of 1,2,3-Trichlorobenzene = 3,779.6 moles
- Mass of 1,2,3-Trichlorobenzene = 3,779.6 moles × 181.4 g/mol = 685.34 kg
- Mass of Nitric Acid = 3,779.6 moles × 63.01 g/mol = 238.11 kg

Step 2 (1,2,3-Trichloro-4-nitrobenzene to 2,3-Dichloro-6-nitroaniline):

- Moles of Ammonia = 3,779.6 moles
- Mass of Ammonia = 3,779.6 moles × 17.03 g/mol = 64.35 kg
- Mass of HCl produced = 3,779.6 moles × 36.46 g/mol = 137.79 kg

Step 3 (2,3-Dichloro-6-nitroaniline to Aclonifen):

- Moles of Phenol = 3,779.6 moles
- Mass of Phenol = 3,779.6 moles × 94.11 g/mol = 355.44 kg
- Mass of HCl produced = 3,779.6 moles × 36.46 g/mol = 137.79 kg

Total Byproduct: HCl: 137.79 kg (Step 2) + 137.79 kg (Step 3) = 275.58 kg

The mass balance in detail is listed in Table 2.

Table 2. Mass balance of aclonifen.

Input (kg)		Output (kg)		Remarks
1,2,3-Trichlorobenzene	685.34	Aclonifen	1000	Product
Phenol	355.44	Toluene	2900	Recovered
Ammonia	64.35	Toluene	100	Loss
Nitric Acid 70%	357	Isopropyl alcohol	1950	Recovered
Toluene	3000	Isopropyl alcohol	50	Loss
Water	8000	Spent sulfuric acid	857	
Sulfuric acid 98%	500	Salt	219.07	To TSDF
NaOH 48%	325	Effluent	8000	To ETP
Isopropyl alcohol	2000	Residue	211.06	Rule 9
Total	15287.13	Total	15287.13	-

AMETRYN CAS# 834-12-8

Manufacturing Process

Atrazine reacts with Sodium methanethiolate to form Ametryn.

Basic Chemistry

Atrazine (MF: C₈H₁₄ClN₅ MW: 215.68 g/mol) reacts with Sodium methanethiolate (MF: CH₃NaS

MW: 70.09 g/mol) to form Ametryn (MF: C₉H₁₇N₅S MW: 227.33 g/mol), as product and NaCl as byproduct (Figure 4).

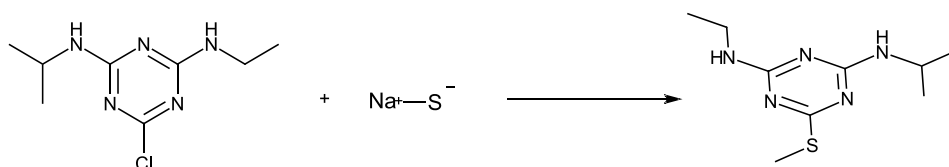
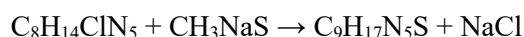


Figure 4. Atrazine reacts with sodium methanethiolate to form ametryn.

Molecular Weights

- Atrazine (C₈H₁₄ClN₅): 215.68 g/mol
- Sodium methanethiolate (CH₃NaS): 70.09 g/mol
- Ametryn (C₉H₁₇N₅S): 227.33 g/mol
- Sodium chloride (NaCl): 58.44 g/mol

Moles of Ametryn to Produce 1 t:

To find the moles of Ametryn for 1 t (1000 kg):

Since the reaction is 1:1, the moles of Atrazine and Sodium methanethiolate required are also 4398.403 moles.

$$\text{Moles of Ametryn} = \frac{\text{Mass of Ametryn}}{\text{Molecular Weight of Ametryn}} = \frac{1000 \text{ kg} \times 1000 \text{ g/kg}}{227.33 \text{ g/mol}} = 4398.403 \text{ moles}$$

Mass of Atrazine: 4398.403 moles × 215.68 g/mol = 948,593.3 g = 948.59 kg

Mass of Sodium methanethiolate: 4398.403 moles × 70.09 g/mol = 307,935.29 g = 307.94 kg

Byproduct (NaCl) Calculation: 4398.403 moles × 58.44 g/mol = 256.53 kg

Mass of solvent = 13,195.209 moles × 92.14 g/mol = 1,215,597.73 g = 1,215.60 kg

The mass balance in detail is listed in Table 3.

Table 3. Mass balance of ametryn.

Input (kg)		Output (kg)		Remarks
Atrazine	948.59	Ametryn	1000	Product
Sodium methanethiolate	307.94	NaCl	256.53	By-Product
Toluene	2500	Toluene	2425	Recovered
Water	4000	Toluene	75	Loss
-	-	Effluent	4000	To ETP
-	-	Salt	-	To TSDF
-	-	Residue	-	Rule 9
Total	7756.53	Total	7756.53	-

AMIDOSULFURON CAS 120923-37-7

Manufacturing Process

N-Methyl-N-sulfamoylmethanesulfonamide reacts with phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate to form Amidosulfuron.

Basic Chemistry

N-Methyl-N-sulfamoylmethanesulfonamide (MF: C₂H₈N₂O₄S₂ MW: 188.23 g/mol) reacts with phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate (MF: C₁₃H₁₃N₃O₄ MW: 275.26 g/mol) to form Amidosulfuron (MF: C₉H₁₅N₅O₇S₂ MW: 369.4 g/mol) and phenol as a byproduct (Figure 5).

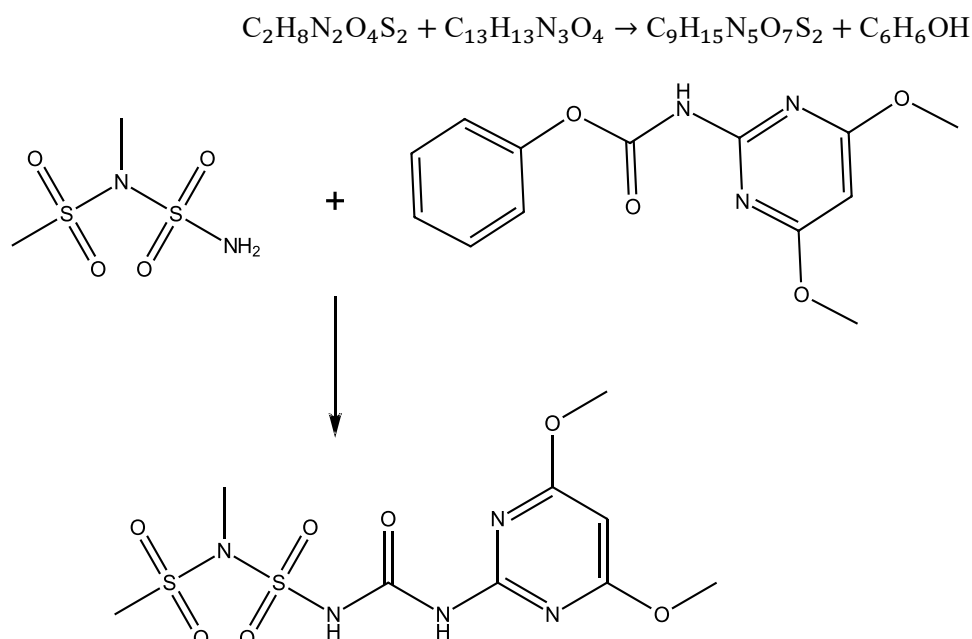


Figure 5. N-Methyl-N-sulfamoylmethanesulfonamide reacts with phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate to form Amidosulfuron.

Reactants

- N-Methyl-N-sulfamoylmethanesulfonamide ($\text{C}_2\text{H}_8\text{N}_2\text{O}_4\text{S}_2$): MW=188.23 g/mol
- Phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate ($\text{C}_{13}\text{H}_{13}\text{N}_3\text{O}_4$): MW=275.26 g/mol
- Amidosulfuron ($\text{C}_9\text{H}_{15}\text{N}_5\text{O}_7\text{S}_2$): MW=369.4 g/mol
- Phenol ($\text{C}_6\text{H}_6\text{O}$): MW=94.11 g/mol

Byproducts: Phenol ($\text{C}_6\text{H}_6\text{O}$) is the primary byproduct.

Calculation of Mass Balance

Moles of Amidosulfuron:

- MW of Amidosulfuron =369.4 g/mol
- Moles of Amidosulfuron in 1 t:

$$\text{Moles of Amidosulfuron} = \frac{1000 \text{ kg}}{369.4 \text{ g/mol}} = 2706.14 \text{ moles}$$

Step-wise Reactant Quantities

N-methyl-N-sulfamoylmethanesulfonamide ($\text{C}_2\text{H}_8\text{N}_2\text{O}_4\text{S}_2$):

- Moles required =2706.14 moles
- Mass required =2706.14 moles×188.23 g/mol=509.52 kg
- Phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate ($\text{C}_{13}\text{H}_{13}\text{N}_3\text{O}_4$):
- Moles required =2706.14 moles
- Mass required =2706.14 moles×275.26 g/mol=745.12 kg

Byproducts

Phenol ($\text{C}_6\text{H}_6\text{O}$):

- Moles produced =2706.14 moles

Mass of phenol =2706.14 moles×94.11 g/mol=254.64 kg

Solvent (Acetone, Toluene, or Ethyl Acetate): ≈2 t.

The mass balance in detail is listed in Table 4.

Table 4. Mass balance of amidosulfuron.

Input (kg)		Output (kg)		Remarks
N-methyl-N-sulfamoylmethane-sulfonamide	509.52	Amidosulfuron	1000	Product
Phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate	745.12	Phenol	254.64	Byproduct
Toluene	2500	Toluene	2450	Recovered
Water	4000	Toluene	50	Loss
-	-	Effluent	4000	To ETP
-	-	Salt	-	To TSDF
-	-	Residue	-	Rule 9
Total	7754.64	Total	7754.64	-

AMINOCYCLOPYRACHLOR CAS 858956-08-8

Manufacturing Process

5,6-dichloro-2-cyclopropylpyrimidine-4-carboxylic acid react in the presence of ammonia to form Aminocyclopyrachlor.

Basic Chemistry

5,6-dichloro-2-cyclopropylpyrimidine-4-carboxylic acid (MF: C₈H₆Cl₂N₂O₂ MW: 233.05 g/mol) reacts in the presence of ammonia (MF: H₃N MW: 17.031 g/mol) to form Aminocyclopyrachlor (MF: C₈H₈ClN₃O₂ MW: 213.62 g/mol) and HCl as a byproduct (Figure 6).

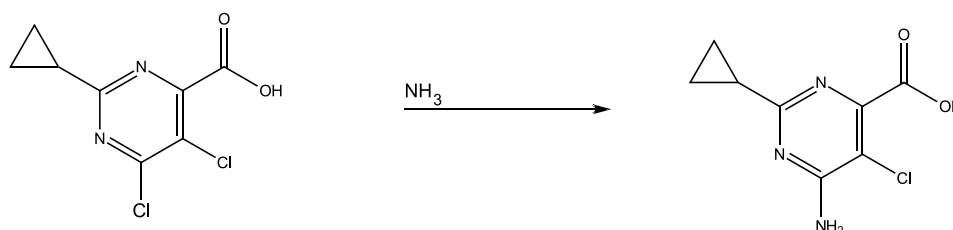
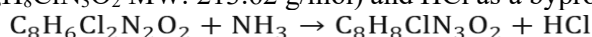


Figure 6. 5,6-dichloro-2-cyclopropylpyrimidine-4-carboxylic acid reacts in the presence of ammonia to form aminocyclopyrachlor.

Reactants

- 5,6-Dichloro-2-cyclopropylpyrimidine-4-carboxylic acid (C₈H₆Cl₂N₂O₂): MW=233.05 g/mol
- Ammonia (NH₃): MW=17.03 g/mol
- Aminocyclopyrachlor (C₈H₈ClN₃O₂): MW=213.62 g/mol
- Hydrochloric Acid (HCl): MW=36.46 g/mol

Calculation of Mass Balance

Moles of Aminocyclopyrachlor:

- MW of aminocyclopyrachlor =213.62 g/mol
- Moles of aminocyclopyrachlor in 1 t:

$$\text{Moles of Aminocyclopyrachlor} = \frac{1000 \text{ kg}}{213.62 \text{ g/mol}} = 4682.54 \text{ moles}$$

Step-Wise Reactant Quantities

5,6-Dichloro-2-cyclopropylpyrimidine-4-carboxylic acid:

- Moles required =4682.54 moles
 - Mass required =4682.54 moles×233.05 g/mol=1091.26 kg
- Ammonia (NH₃):

- Moles required = 4682.54 moles
- Mass required = 4682.54 moles × 17.03 g/mol = 79.74 kg

Byproducts: Hydrochloric Acid (HCl):

- Moles produced = 4682.54 moles
- Mass of HCl = 4682.54 moles × 36.46 g/mol = 170.77 kg

Solvent (Ethanol, Methanol, Acetonitrile, or DMF): ~2.1 t.

The mass balance in detail is listed in Table 5.

Table 5. Mass balance of aminocyclopyrachlor.

Input (kg)		Output (kg)		Remarks
5,6-Dichloro-2-cyclopropylpyrimidine-4-carboxylic acid	1091.79	Aminocyclopyrachlor	1000	Product
Ammonia	79.74	HCl	569	Rule 9
Ethanol	2100	Ethanol	2050	Recovered
Water	3500	Ethanol	50	Loss
Water for HCl	398	Effluent	3500	To ETP
-	-	Salt	-	To TSDF
-	-	Residue	-	Rule 9
Total	7169	Total	7169	-

AMINOPYRALID CAS 150114-71-9

Manufacturing Process

The formation of Aminopyralid from 4-amino-3,5,6-trichloropyridine-2-carboxylic acid through a hydrogenation reaction in the presence of a Pt-C catalyst and hydrogen gas (H₂).

Basic Chemistry

Formation of 4-amino-3,6-dichloropyridine-2-carboxylic acid, known as Aminopyralid (MF: C₆H₄Cl₂N₂O₂, MW: 207.01 g/mol), from 4-amino-3,5,6-trichloropyridine-2-carboxylic acid (MF: C₆H₃Cl₃N₂O₂, MW: 241.5 g/mol) through a hydrogenation reaction in the presence of a Pt-C catalyst and hydrogen gas (H₂). HCl is a byproduct (Figure 7).

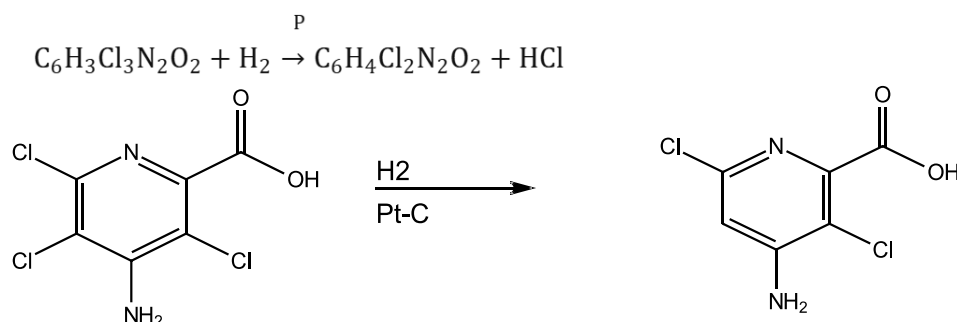


Figure 7. Route of synthesis of aminopyralid.

Reactants

- 4-Amino-3,5,6-trichloropyridine-2-carboxylic acid (C₆H₃Cl₃N₂O₂): MW=241.50 g/mol
- Hydrogen gas (H₂): MW=2.016 g/mol
- Aminopyralid (4-Amino-3,6-dichloropyridine-2-carboxylic acid) (C₆H₄Cl₂N₂O₂): MW=207.01 g/mol
- Hydrochloric acid (HCl): MW=36.46 g/mol

Calculation of Mass Balance

Moles of Aminopyralid:

- MW of Aminopyralid = 207.01 g/mol
- Moles of Aminopyralid in 1 t:

$$\text{Moles of Aminopyralid} = \frac{1000 \text{ kg}}{207.01 \text{ g/mol}} = 4831.61 \text{ moles}$$

Step-Wise Reactant Quantities

4-Amino-3,5,6-trichloropyridine-2-carboxylic acid:

- Moles required = 4831.61 moles
- Mass required = 4831.61 moles × 241.50 g/mol = 1166.26 kg

Hydrogen gas (H₂):

- Moles required = 4831.61 moles
- Mass required = 4831.61 moles × 2.016 g/mol = 9.74 kg

By-products: Hydrochloric Acid (HCl):

- Moles produced = 4831.61 moles
- Mass of HCl = 4831.61 moles × 36.46 g/mol = 176.12 kg

The mass balance in detail is listed in Table 6.

Table 6. Mass balance of aminopyralid.

Input (kg)		Output (kg)		Remarks
4-Amino-3,5,6-trichloropyridine-2-carboxylic acid	1166.26	Aminopyralid	1000	Product
Hydrogen gas	9.74	HCl	585	Rule 9
Ethanol	2000	Ethanol	1950	Recovered
Water	3500	Ethanol	50	Loss
Water for HCl	409	Spent catalyst	20	
Catalyst	20	Effluent	3500	To ETP
-	-	Salt	-	To TSDF
-	-	Residue	-	Rule 9
Total	7105	Total	7105	-

ATRAZINE CAS# 1912-24-9

Manufacturing Process of Atrazine

Step-1: Cynuric chloride was reacted with isopropyl amine in the presence of NaOH to neutralize HCl in toluene as a solvent to give 4,6-dichloro-N-isopropyl-1,3,5-triazin-2-amine, which was in toluene and used for the next step.

Step-2: 4,6-dichloro-N-isopropyl-1,3,5-triazin-2-amine was further reacted with ethyl amine in the presence of NaOH to neutralize HCl and toluene as a solvent medium. This mass was further concentrated and filtered to afford Atrazine technical (Figure 8).

Chemical Reaction

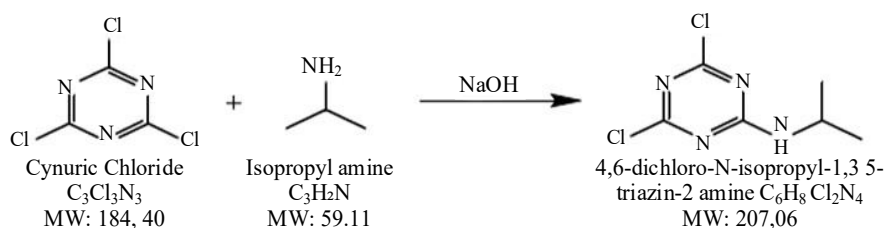
Raw Material

- Cynuric Chloride
- Isopropyl amine
- 47% NaOH
- Ethyl amine

- Toluene
- Water
- Ejector Water
- Scrubber water

The mass balance in detail is listed in Table 7.

Step-1



Step-2

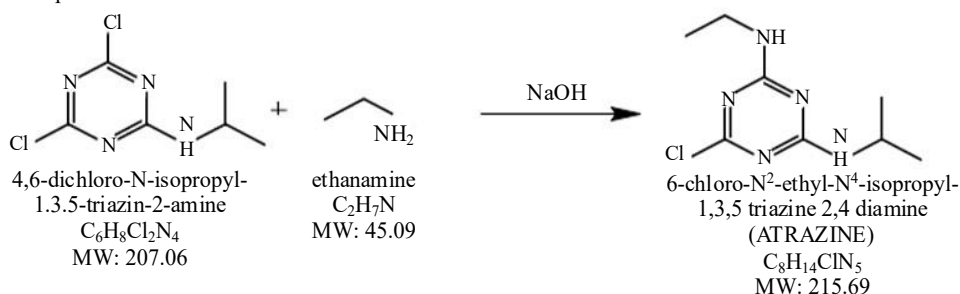


Figure 8. Route of synthesis of atrazine.

Table 7. Mass balance of atrazine.

Input (kg)		Output (kg)	
Cyanuric Chloride	950	Atrazine	1000
Isopropyl amine	370	Recovered Toluene Reuse	3090
47% NaOH	849	Toluene Loss	110
Ethyl amine	230	Effluent (ETP)	2000
Toluene	3200	Ejector Water (ETP)	2000
Water	2000	Caustic lye water (ETP)	450
Ejector Water	2000	Scrubber water (MEE)	2000
Scrubber water	2000	Amine water (in starting RM)	180
-	-	Sodium chloride salt (TSDF)	573
-	-	Organic impurity (TSDF)	196
Total	11599	Total	11599

AZIMSULFURON CAS# 120162-55-2

Manufacturing Process

2-methyl-4-(2-methyltetrazol-5-yl) pyrazole-3-sulfonamide reacts with phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate to form Azimsulfuron.

Basic Chemistry

2-methyl-4-(2-methyltetrazol-5-yl) pyrazole-3-sulfonamide (MF: C₆H₉N₇O₂S MW: 243.25 g/mol) reacts with phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate (MF: C₁₃H₁₃N₃O₄ MW: 275.26 g/mol)

to form azimsulfuron (MF: C₁₃H₁₆N₁₀O₅S MW: 424.4 g/mol) and phenol as a byproduct (Figure 9).

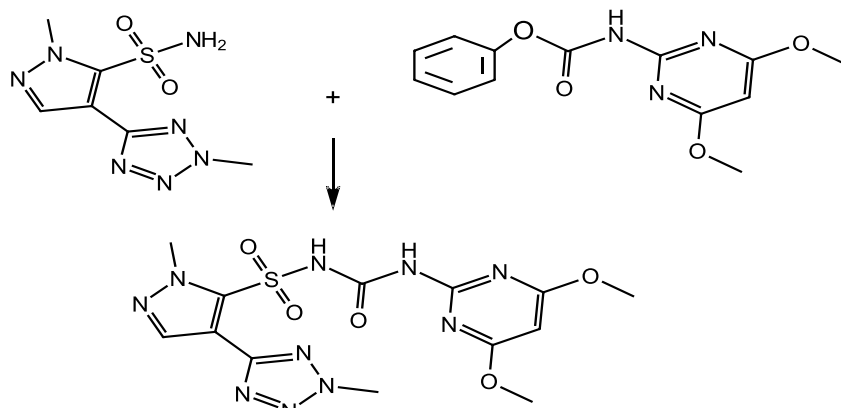
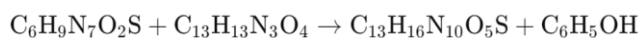


Figure 9. 2-methyl-4-(2-methyltetrazol-5-yl) pyrazole-3-sulfonamide reacts with phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate to form azimsulfuron.

Reactants

- 2-Methyl-4-(2-methyltetrazol-5-yl) pyrazole-3-sulfonamide (C₆H₉N₇O₂S): MW=243.25 g/mol
- Phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate (C₁₃H₁₃N₃O₄): MW=275.26 g/mol
- Azimsulfuron (C₁₃H₁₆N₁₀O₅S): MW=424.40 g/mol
- Phenol (C₆H₆O): MW=94.11 g/mol (by-product)

Calculation of Mass Balance

Moles of Azimsulfuron:

- MW of azimsulfuron =424.40 g/mol
- Moles of azimsulfuron in 1 t:

$$\text{Moles of Azimsulfuron} = \frac{1000 \text{ kg}}{424.40 \text{ g/mol}} = 2356.36 \text{ moles}$$

Step-Wise Reactant Quantities

2-Methyl-4-(2-methyltetrazol-5-yl) pyrazole-3-sulfonamide:

- Moles required =2356.36 moles
- Mass required =2356.36 moles×243.25 g/mol=573.29 kg

Phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate:

- Moles required =2356.36 moles
- Mass required =2356.36 moles×275.26 g/mol=648.46 kg

Table 8. Mass balance of azimsulfuron.

Input (kg)		Output (kg)		Remarks
2-Methyl-4-(2-methyltetrazol-5-yl) pyrazole-3-sulfonamide	573.29	Azimsulfuron	1000	Product
Phenyl N-(4,6-dimethoxypyrimidin-2-yl) carbamate	648.46	Phenol	221.75	By-Product
Toluene	3000	Toluene	2900	Recovered
Water	4000	Toluene	100	Loss
-	-	Effluent	4000	To ETP
-	-	Salt	-	To TSDF
-	-	Residue	-	Rule 9
Total	8221.75	Total	8221.75	-

Byproduct: Phenol:

- Moles produced=2356.36 moles
- Mass of phenol=2356.36 moles×94.11 g/mol=221.75 kg

The mass balance in detail is listed in Table 8.

BEFLUBUTAMID CAS 113614-08-7

Manufacturing Process

Ethyl 2-[4-fluoro-3-(trifluoromethyl) phenoxy] butanoate reacts with benzylamine to form beflubutamid (Figure 10).

Basic Chemistry

Ethyl 2-[4-fluoro-3-(trifluoromethyl) phenoxy] butanoate (MF: C₁₃H₁₄F₄O₃ MW: 294.24 g/mol) reacts with benzylamine (MF: C₇H₉N MW: 107.15 g/mol) to form beflubutamid (MF: C₁₈H₁₇F₄NO₂ MW: 355.3 g/mol) and ethanol as a byproduct.

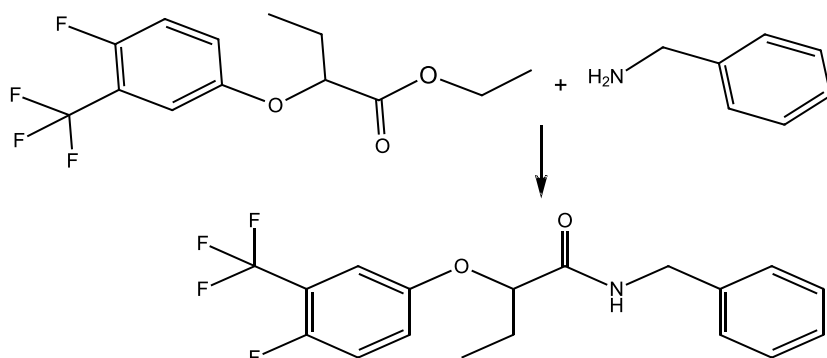
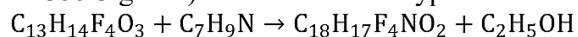


Figure 10. Route of synthesis of beflubutamid.

Reactants and Product

- Ethyl 2-[4-fluoro-3-(trifluoromethyl) phenoxy]butanoate (C₁₃H₁₄F₄O₃): MW=294.24 g/mol
- Benzylamine (C₇H₉N): MW=107.15 g/mol
- Beflubutamid (C₁₈H₁₇F₄NO₂): MW=355.3 g/mol
- Ethanol (C₂H₅OH): MW=46.07 g/mol (byproduct)

Calculation of Mass Balance

Moles of Beflubutamid:

- MW of beflubutamid =355.3 g/mol
 - Moles of beflubutamid in 1 t:
- $$\text{Moles of Beflubutamid} = \frac{1000 \text{ kg}}{355.3 \text{ g/mol}} = 2814.47 \text{ moles}$$

Step-Wise Reactant Quantities

Ethyl 2-[4-fluoro-3-(trifluoromethyl)phenoxy] butanoate:

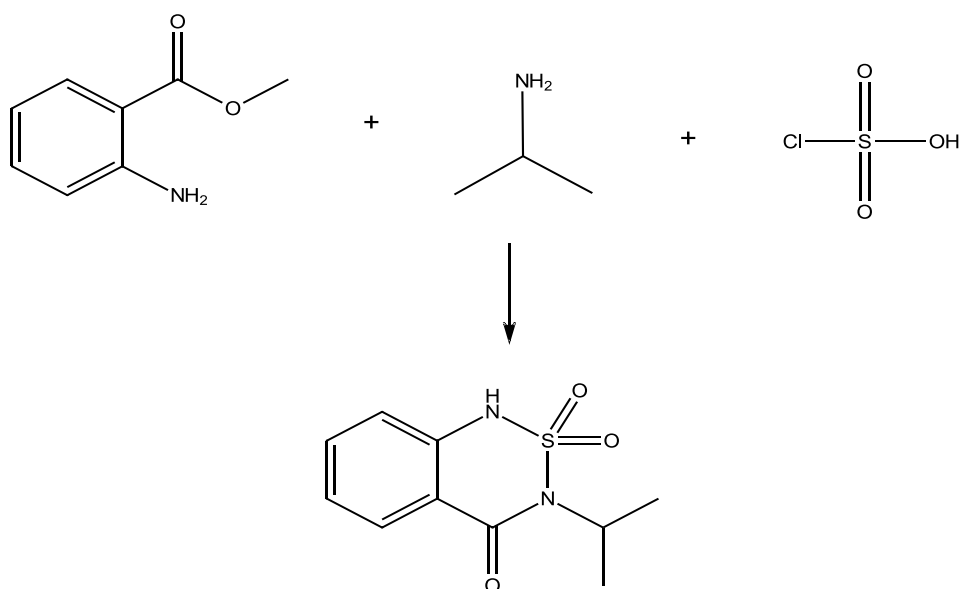
- Moles required =2814.47 moles
- Mass required =2814.47 moles×294.24 g/mol=827.78 kg

Benzylamine:

- Moles required =2814.47 moles
- Mass required =2814.47 moles×107.15 g/mol=301.58 kg

Table 10. Mass balance of bensulfuron.

Input (kg)		Output (kg)		Remarks
4,6-Dimethoxy Pyrimidine-2-Amine	418	Bensulfuron	1000	Product
Methyl-2-[[Isocyanate sulfamoyl] Methyl] Benzoate	620	Xylene	1500	Recovered
Xylene	1600	Xylene	100	Loss
Methanol	2000	Methanol	1900	Recovered
Water	2000	Methanol	100	Loss
-	-	Effluent	2000	To ETP
-	-	Residue	38	Rule 9
-	-	Salt	-	To TSDF
Total	6638	Total	6638	-

**Figure 12.** Chemical Reaction to form bentazone.**Raw Material**

- Amino Benzoic Acid
- Isopropyl Amine
- Chlorosulphonic Acid
- EDC
- Water

The mass balance in detail is listed in Table 11.

Table 11. Mass balance of bentazone.

Input (kg)		Output (kg)		Remarks
Amino Benzoic Acid	741	Bentazone	1000	Product
Isopropyl Amine	304	HCl 30%	593	Rule 9
Chlorosulphonic Acid	628	Recovery EDC	2046	Recovered
EDC	2223	Loss EDC	177	Loss
Water	1500	Methanol	158	By-Product
Water for HCl	415	Aqueous Waste	1837	-
Total	5811	Total	5811	-

CONCLUSION

The synthesis and production of the 10 high-volume herbicides analyzed in this study demonstrate the complexity and diversity of chemical processes in the agrochemical industry. The detailed mass balance calculations reveal the significant quantities of raw materials, solvents, and byproducts involved, highlighting the importance of efficient resource utilization and waste management. Byproducts such as hydrochloric acid, sodium chloride, and phenol, along with solvent recovery and effluent treatment, pose environmental challenges that require careful handling to comply with regulatory standards. The stoichiometric and mass balance data provided offer valuable insights for optimizing production efficiency, reducing waste, and minimizing environmental impact. Future research should focus on developing greener synthesis routes, improving solvent recovery systems, and exploring alternatives to hazardous byproducts to enhance the sustainability of herbicide production.

REFERENCES

1. American Chemical Society. Guidelines for chemical process safety and environmental protection. Washington, DC: ACS Publications; 2020.
2. Bunch RL, McMullin TS. Advances in herbicide synthesis: Process optimization and environmental considerations. *J Agric Food Chem.* 2018; 66(12): 3005–3012. <https://doi.org/10.1021/acs.jafc.7b05432>
3. European Chemicals Agency. (2023). Registration dossier: Aclonifen (CAS 74070-46-5). [Online]. Retrieved from <https://echa.europa.eu/registration-dossier/-/registered-dossier/12345>
4. Hayes TB, Hansen M. From silent spring to silent night: A review of the environmental impacts of herbicides. *Environ Health Perspect.* 2017; 125(6): 066004. <https://doi.org/10.1289/EHP1417>
5. International Union of Pure and Applied Chemistry. Compendium of chemical terminology. 3rd Edn. Research Triangle Park, NC: IUPAC; 2019.
6. Jeschke P. Progress in herbicide research and development: Chemistry and mode of action. *Pest Manag Sci.* 2016; 72(1): 7–25. <https://doi.org/10.1002/ps.4152>
7. Kraehmer H, van Almsick A. Modern herbicide chemistry: Synthesis and environmental fate. *Weed Sci.* 2021; 69(3): 245–257. <https://doi.org/10.1017/wsc.2020.89>
8. Rao PS, Hornsby AG. Herbicide chemistry and environmental fate. New York, NY: Wiley; 202.
9. Singh SB, Kulshrestha G. Environmental impact of herbicide production: A case study on atrazine and related compounds. *Environ Monitor Assess.* 2020; 192(4): 234. <https://doi.org/10.1007/s10661-020-08188-7>
10. United States Environmental Protection Agency. (2022). Pesticide manufacturing and waste management guidelines. [Online]. Retrieved from <https://www.epa.gov/pesticide-registration/pesticide-manufacturing>
11. World Health Organization. Guidelines for the safe use of pesticides in agriculture. Geneva: WHO Press; 2020.
12. Zhang W, Shan Y. Mass balance and waste minimization in pesticide production. *J Clean Prod.* 2019; 210: 1045–1054. <https://doi.org/10.1016/j.jclepro.2018.11.087>