Multi-Objective Optimization of Dual Reactor Polyethylene Process Using Genetic Algorithms

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Outline

- Introduction
- NOVA Chemicals' Advanced SCLAIRTECH^{TM} Technology
  - Product Design Flexibility
- Multi-objective Optimization: Case Study
  - Genetic Algorithms
- Summary and Conclusions

Polyethylene Applications

- Flexible films
- Injection molded articles
- Roto-molded articles
- Pipes and sheets
- Fibers and artificial turf
- Various other applications

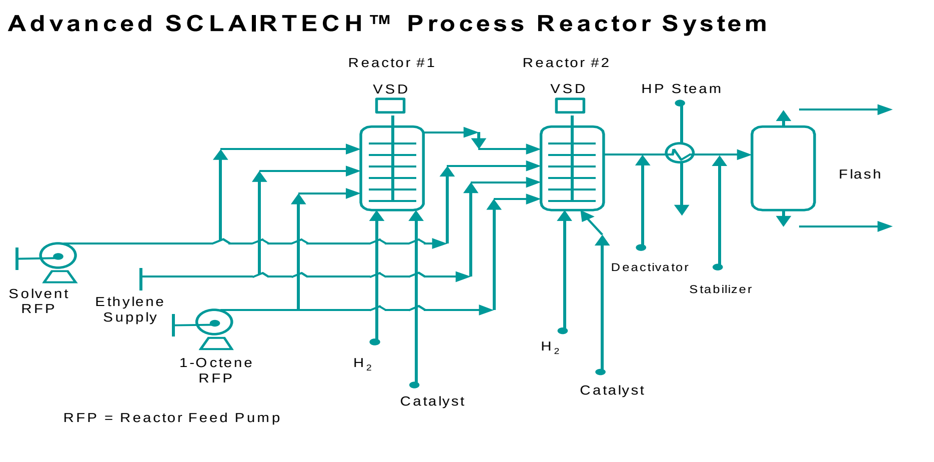
The Performance of PE Resins

- **Physical properties**
  - Type, degree and distribution of branching
  - Molecular weight and molecular weight distribution

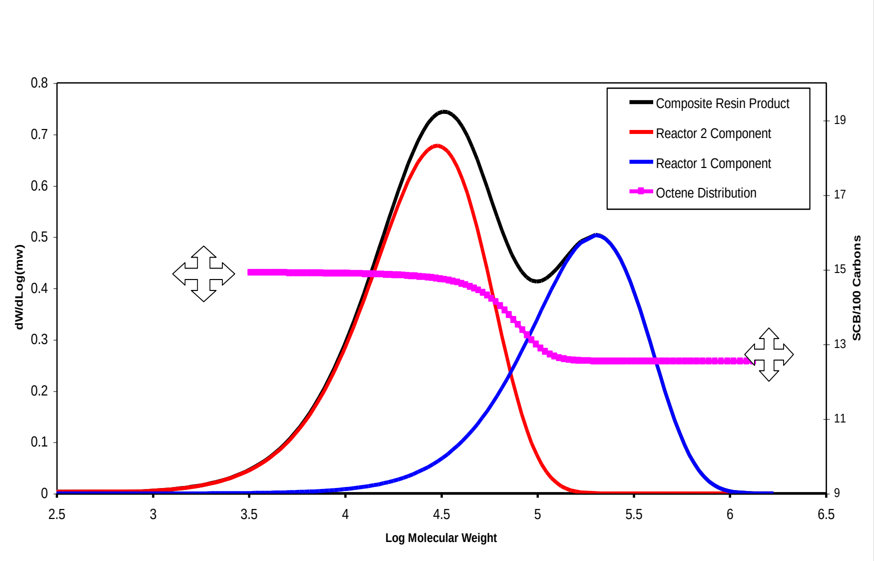
- **Processability**
  - Weight - average molecular weight (melt index)
  - Molecular weight distribution (melt flow ratio)

Dual Reactor Polymerization Process

Use of Dual Reactors



Molecular Design Opportunities



Dual Reactor Process Variables

12 main process variables that affect polymer architecture and production rates:

- R1 and R2 ethylene conversions
- R1 and R2 bulk temperatures
- H_2 amount in R1 and R2
- Ethylene flow split between R1 and R2
- Co-monomer flow split between R1 and R2
- Total Solution Rate (TSR) through both reactors
- Total octene flow
- R1 and R2 inlet flow temperatures

- R1 and R2 indicate first and second reactors.

Process Constraints

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Constraint	Reason
R1 Temperature > Minimum	Polymer precipitation
R2 Temperature > Minimum	Heater capacity
R1 and R2 H2 > Minimum	Gels formation and valve control limits
(R1 + R2) H2 < Maximum	H2 Compressor limit
R2 Octene flow = 0 or > Minimum	Valve control limit
R2 Ethylene % < Maximum	Thermodynamic solubility limit
R1 TSR < Maximum, R2 TSR > Minimum	Mixing, residence time
Ethylene flow out of reactors < Maximum	Recycle valve capacity
Octene flow out of reactors < Maximum	Distillation capacity
Solvent flow out of reactors < Maximum	Distillation capacity

Process Objectives

Maximize Production Rates
Minimize Production Costs
Feasible to Manufacture without Constraints

Case Study:
Cast Film Resin Development




Desired Product Performance Requirements:

- High dart impact strength
- High puncture resistance
- Good processability on cast film lines

Cast Film Resin Development

Desired Product Specifications:

- Melt Index = 4.0 $\pm$ 0.6 (g/10 min)
- Density = 0.9175 $\pm$ 0.0015 g/cc
- Melt Flow Ratio = 21 $\pm$ 2

Product Constraints

Desired Product Structure:

- **Molecular Weight Distribution**
  - Narrow: PD = 2.1 $\pm$ 0.30
- **Co-monomer Distribution**
  - Maximize physical properties
  - Minimize octene requirement
  - Minimize manufacturing costs

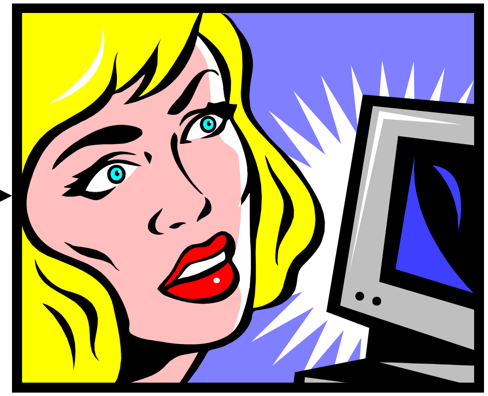
Product Objective

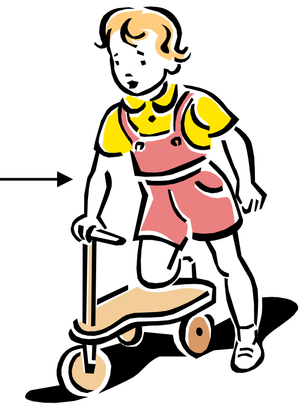
Maximize branch frequency in high molecular weight polymer fraction made in Reactor 1.

Multi- Objective Optimization

- Need both the optimized process and product simultaneously

Multi- objective Optimization: Philosophy





Reactor 1 → Reactor 2 → Product Performance

Reactor 1 → Reactor 2 → Production Rate, Manufacturing Cost

Genetic Algorithms

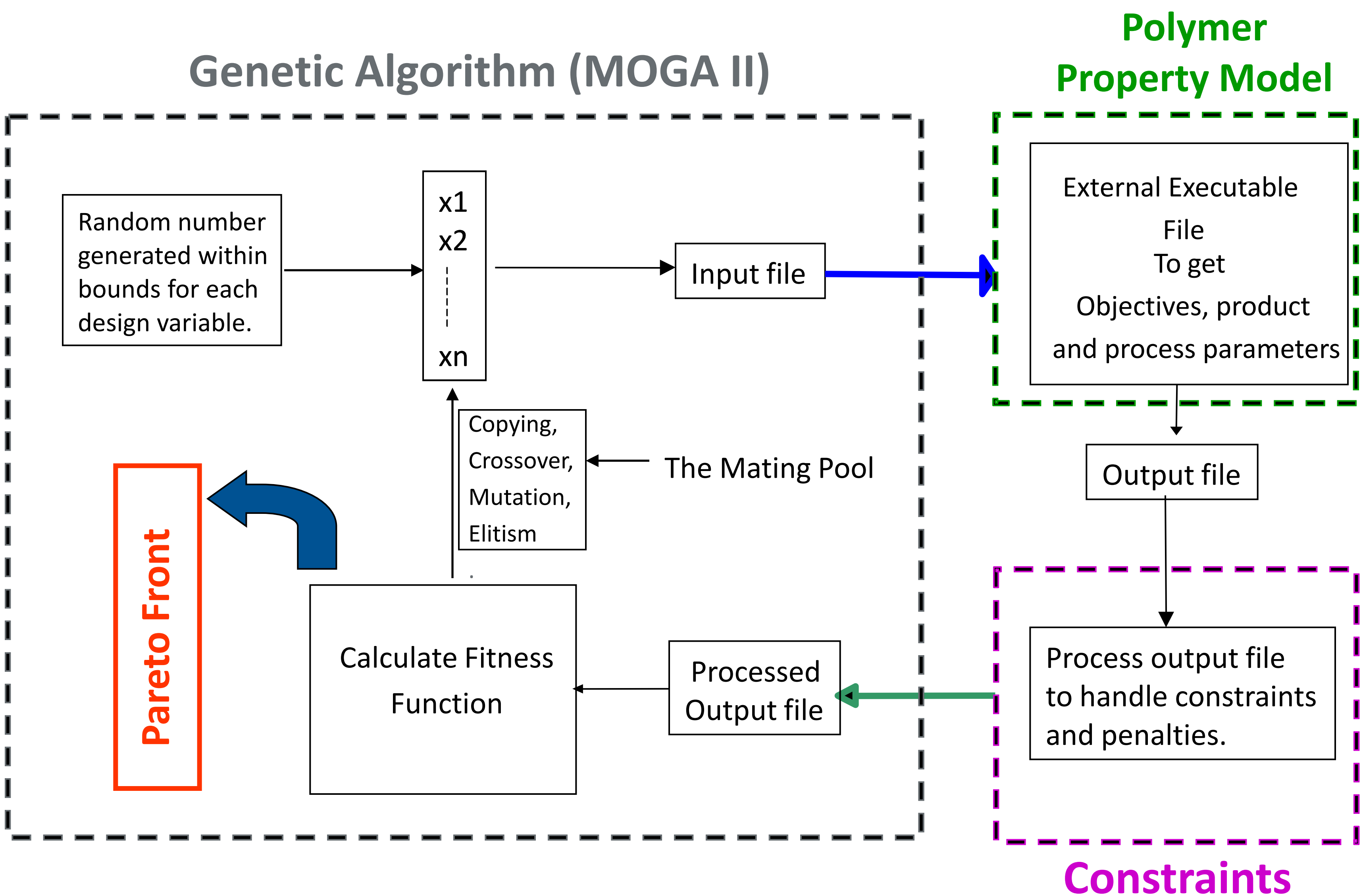
- Genetic Algorithms utilize the concepts of natural selection.

- GAs solve problems by an evolutionary process resulting in better (*fittest*) solutions over successive generations.

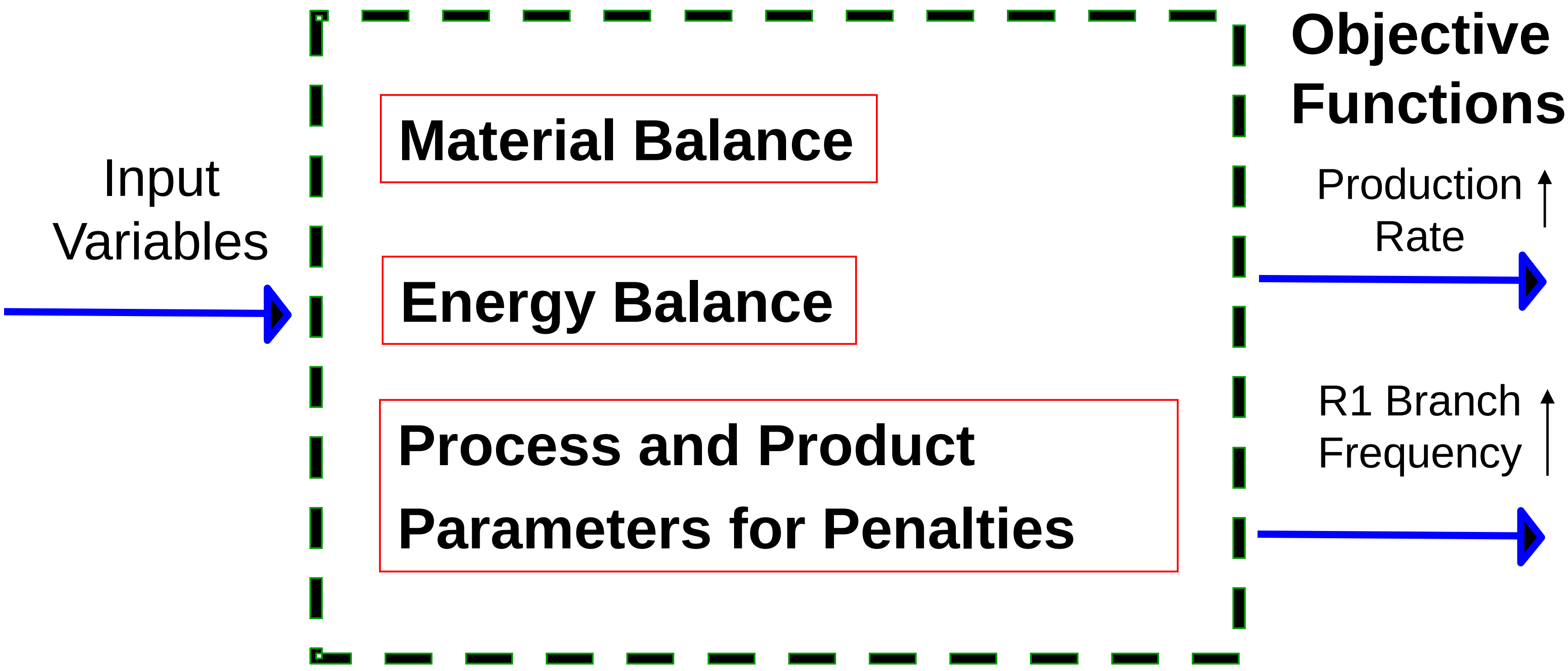
- GAs search from a *population* of points, not based on single point calculations.

- GAs use *fitness functions*, not the objective functions by itself.

Genetic Algorithm (MOGA II)



Polymer Property Model



Fitness Calculation

Product and Process Constraints are handled through the *fitness functions*:

$$f(x) = Obj(x) - \left(r \sum_{i=1}^{K} \left| < \phi_i > \right| + r \sum_{j=1}^{L} \left| < \psi_j > \right| \right)$$

$f(x)$ = Production Rate (or R1 Branch Frequency) with penalties

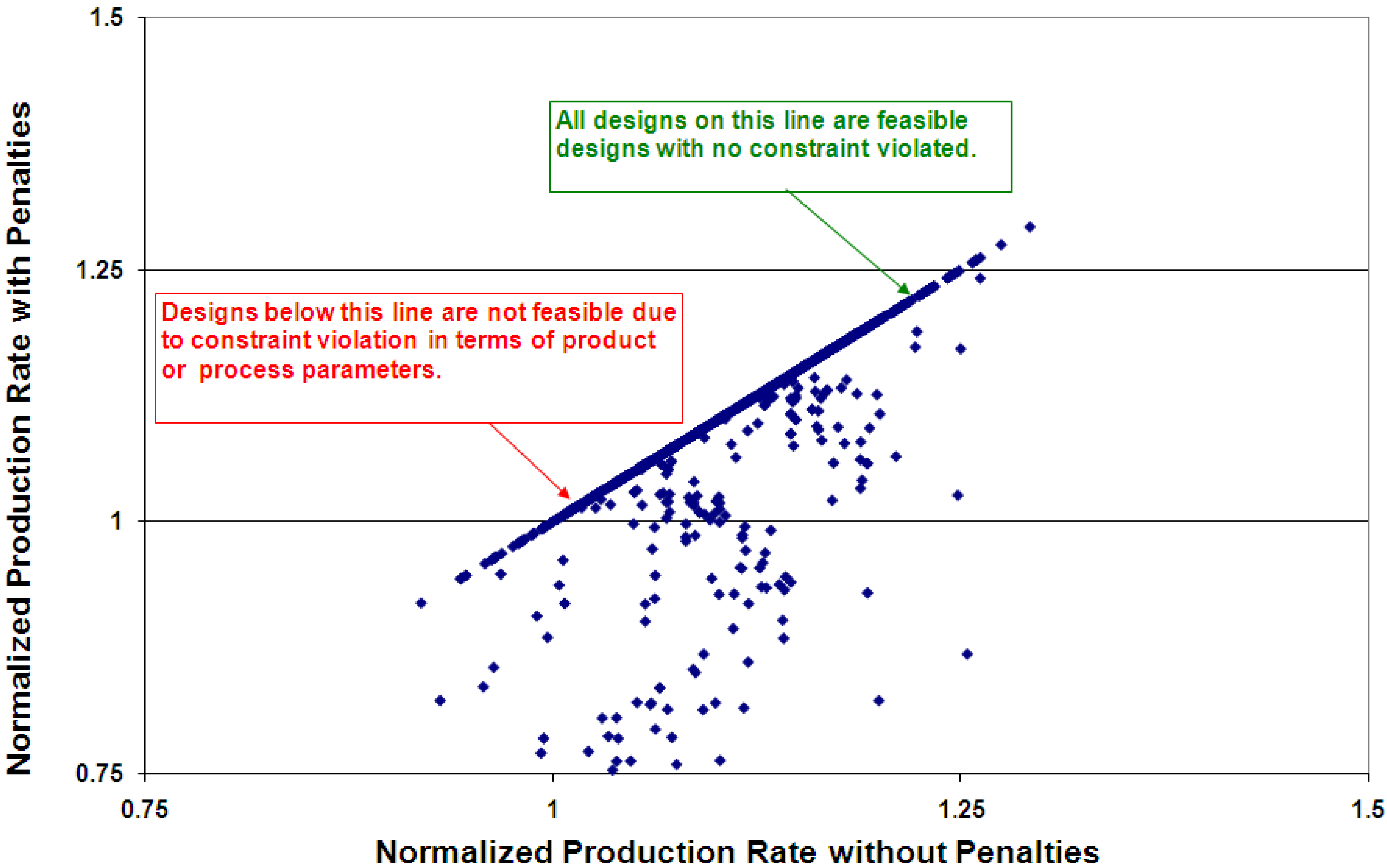
$Obj.(x)$ = Production Rate (or R1 Branch Frequency) *without* penalties

$r \sum_{i=1}^{K} \left| < \phi_i > \right|$ = Weighted Sum of *Process* Penalties

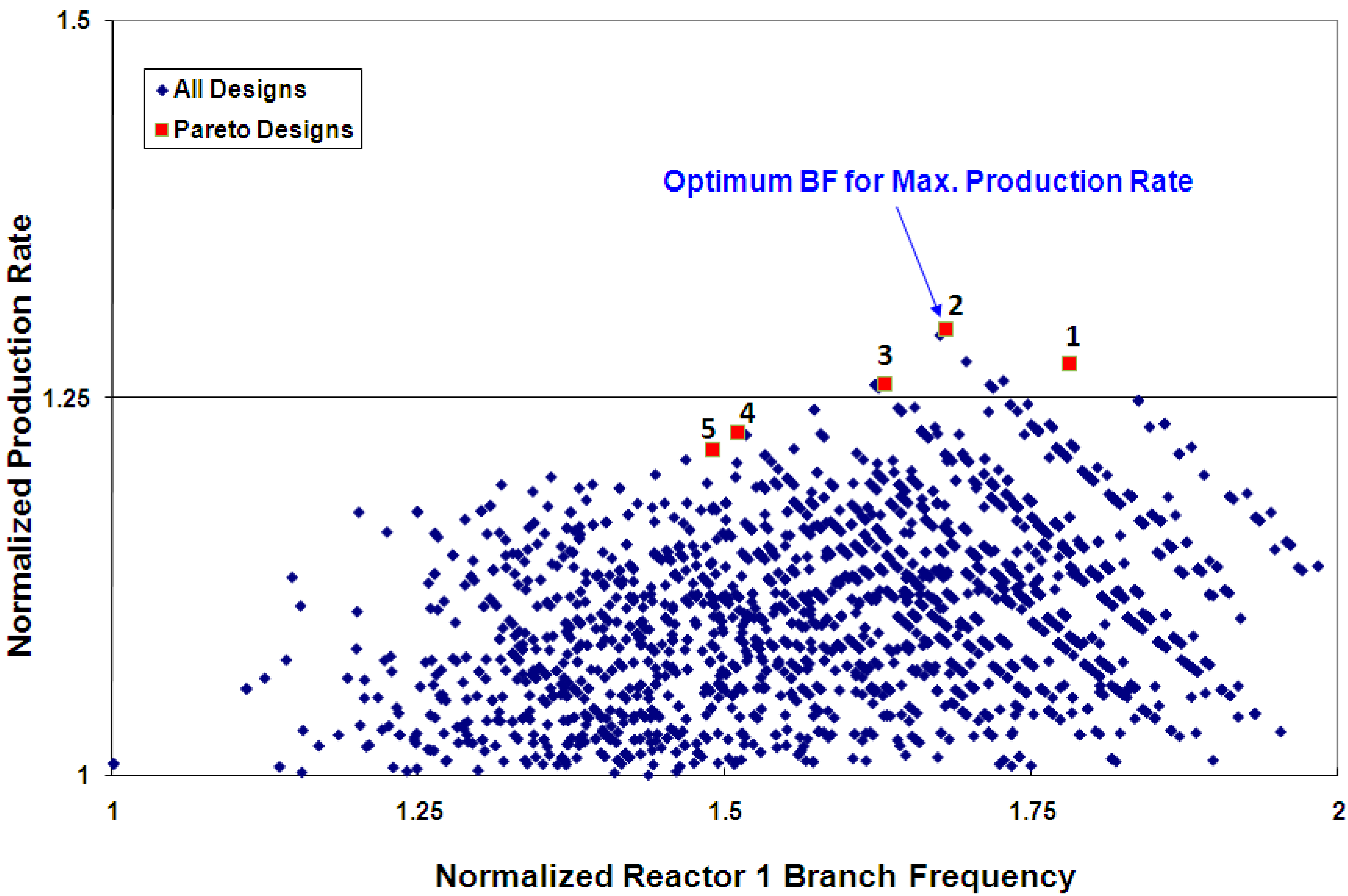
$r \sum_{j=1}^{L} \left| < \psi_j > \right|$ = Weighted Sum of *Product* Penalties

Simulation Results

Normalized Production Rate With and Without Penalties



Production Rate versus Reactor 1 Branch Frequency

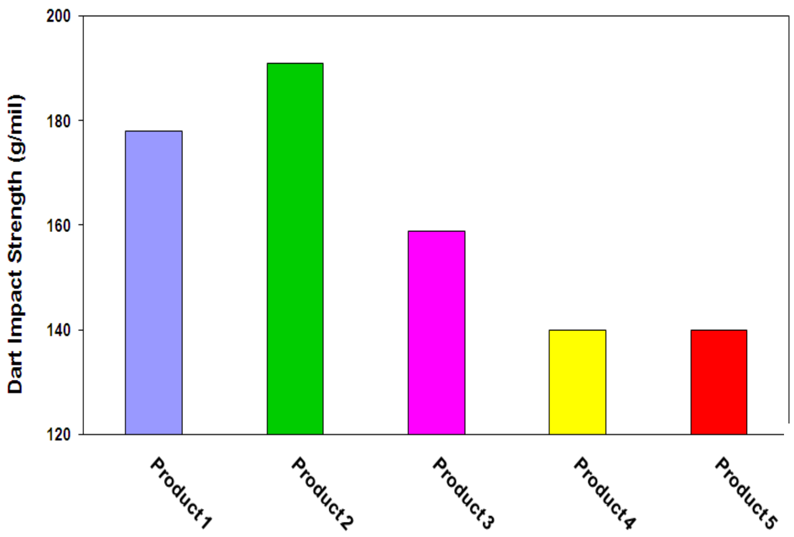


Experimental Validation

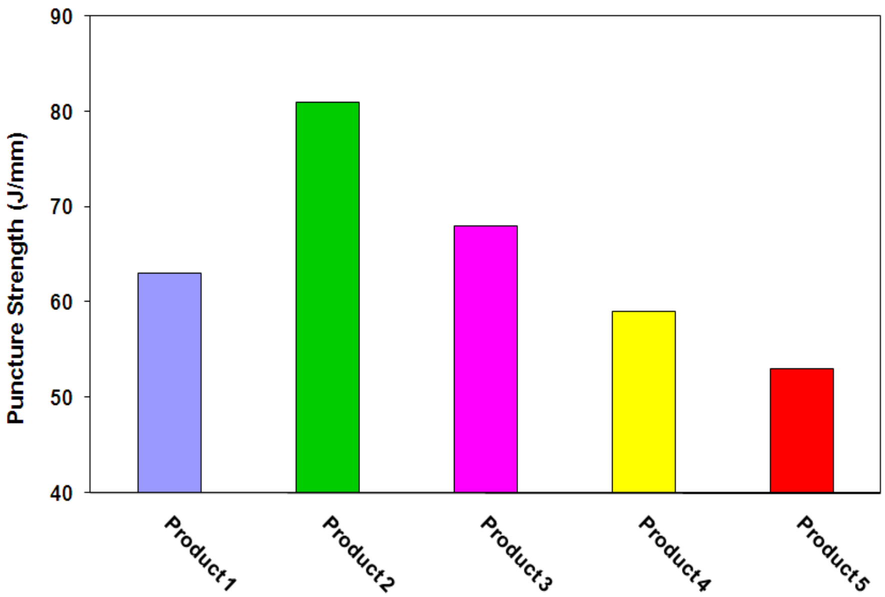
Experimental

- **Pilot plant experiments**
  - Five cast film resins were made with desired product specifications (MI, Density and Melt Flow Ratio).
  - The resins were converted into films using an industrial scale Gloucester cast film line.
  - Physical properties of the films were measured.

Dart Impact Strength of 0.8 mil Cast Films



Puncture Strength of 0.8 mil Cast Films



Scale-up From Pilot Plant to Commercial Plant

- Product # 2 was chosen for scale-up to commercial plant at Joffre, Alberta.
- Demonstrated ~ 20% improvement in production rate
- ~16% reduction in octene requirement
  - Lower variable manufacturing cost (VMC)
- ~10°C increase R2 outlet temperature
  - Lower steam costs resulting in lower VMC
- Demonstrated improved dart impact and puncture strength of the cast films.

Summary and Conclusions

1. NOVA Chemicals' dual reactor Advanced SCLAIRTECH™ Technology provides:
   - New molecular design opportunities
   - Product design flexibility

2. Genetic algorithms can be effectively utilized for multi-objective product- process optimization of the dual reactor polymerization process to improve:
   - Product performance
   - Production rates and manufacturing efficiencies

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