Water Treatment Optimization in a Basin Model for Water Resources Simulation

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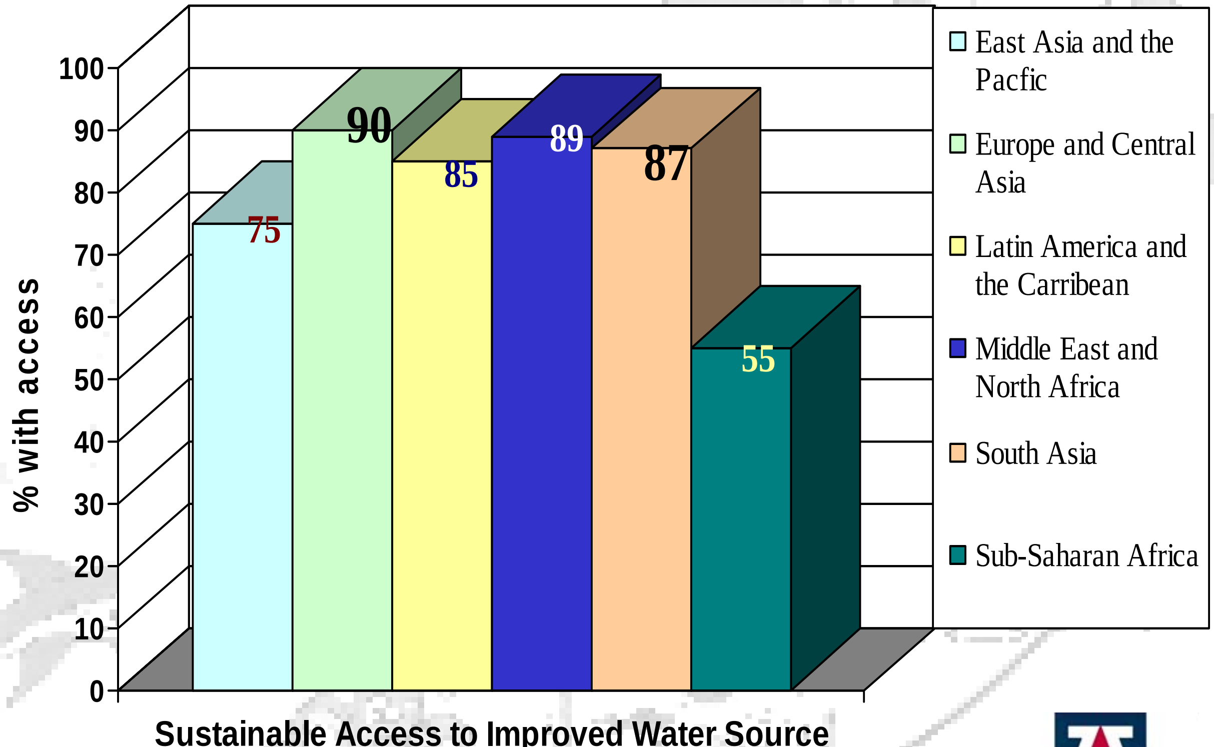
Water Needs for Population and Sustainable Growth Worldwide

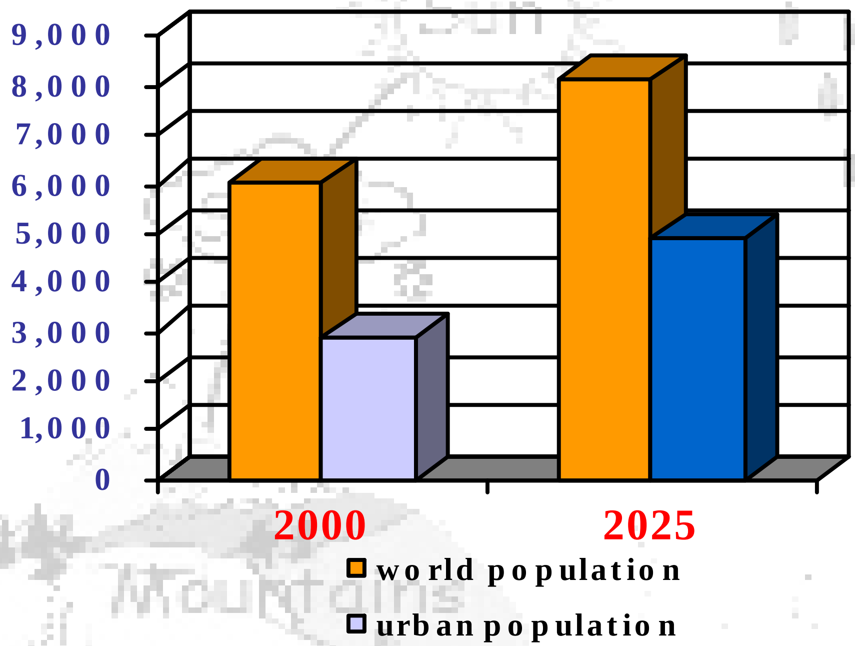
The availability of clean water is already a major issue, and will become a 'water crisis' if we do not act urgently

Access to Water Remains Insufficient, Especially for the Poor

- Access to water is far from being a given, and often over-estimated
- In many parts of the world, access to water also distinguishes the poor from the non-poor



Water Needs for Population and Sustainable Growth Worldwide



- Growing worldwide population
- Most of that population growth is concentrated in urban centers, especially in smaller cities

- In the next 30 minutes, about 180 children in developing countries (six children per minute) will have died from disease caused by unsafe water and inadequate sanitation.
- Water is central for ordinary people in the developing world
- The lack of access to basic services (water and sanitation) and energy (hydropower) hinders growth in the poor countries.

Issues Specific to the Desert Southwest

- Water demand > Available water supply
- Insufficient water quality to meet required uses
- AMA requirement ⇒ supply and demand must be brought in balance by prescribed deadlines
- Alternative measures, such as agricultural land retirement, water transfers, and conservation, are being considered to ease water shortfalls and current drought conditions.

Issues Specific to the Desert Southwest

- Rapidly growing populations in states such as Nevada, Arizona, and California

- No readily available sources of new water supplies in many of these areas

- Drought events debilitate available sources

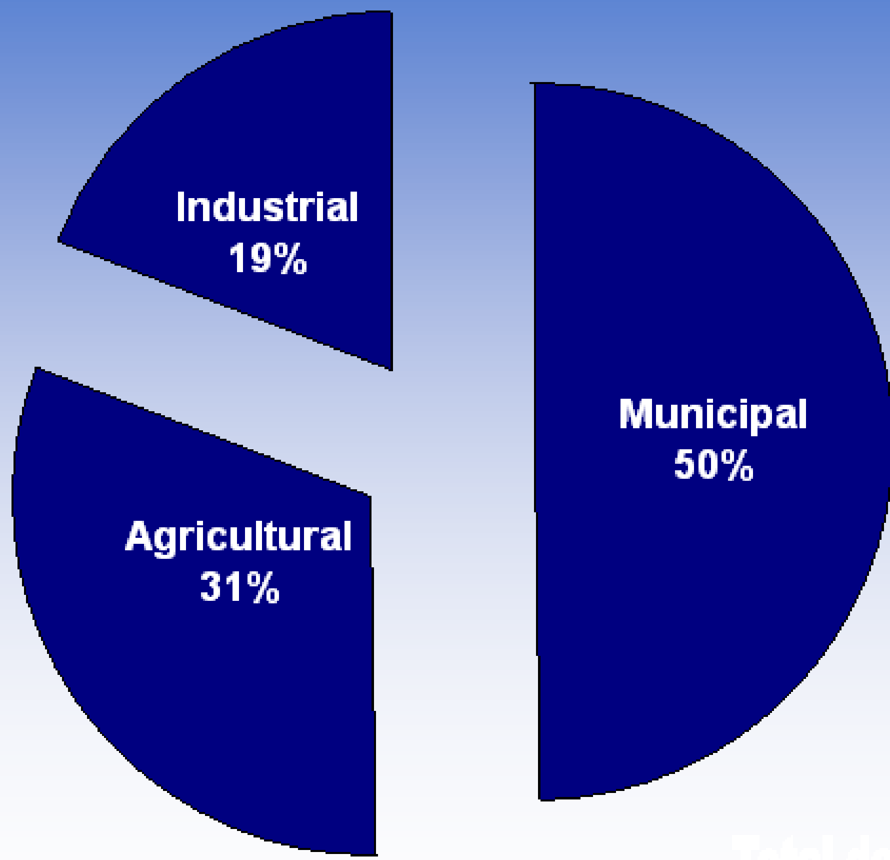
- High costly alternative sources of supply

The possible solution: Reuse of Water

- meets the needs of industrial users for non-potable supply
- solves environmental discharge problems

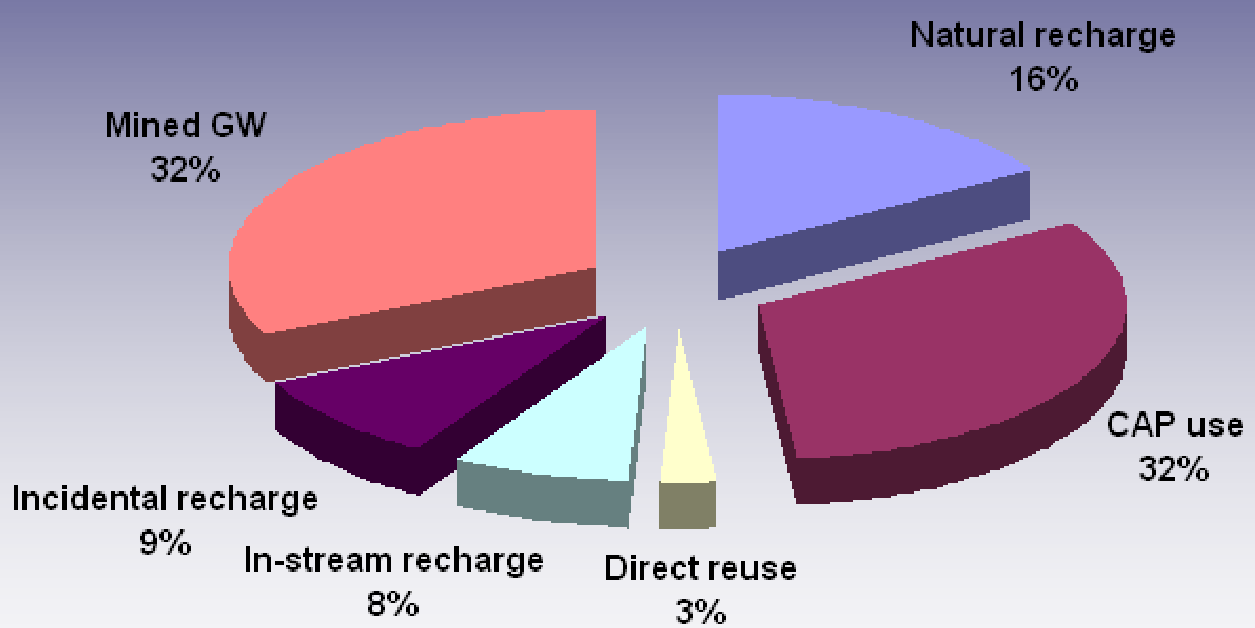

Where did
everybody go?

Water Demand Components in the Tucson Active Management Area (2005)

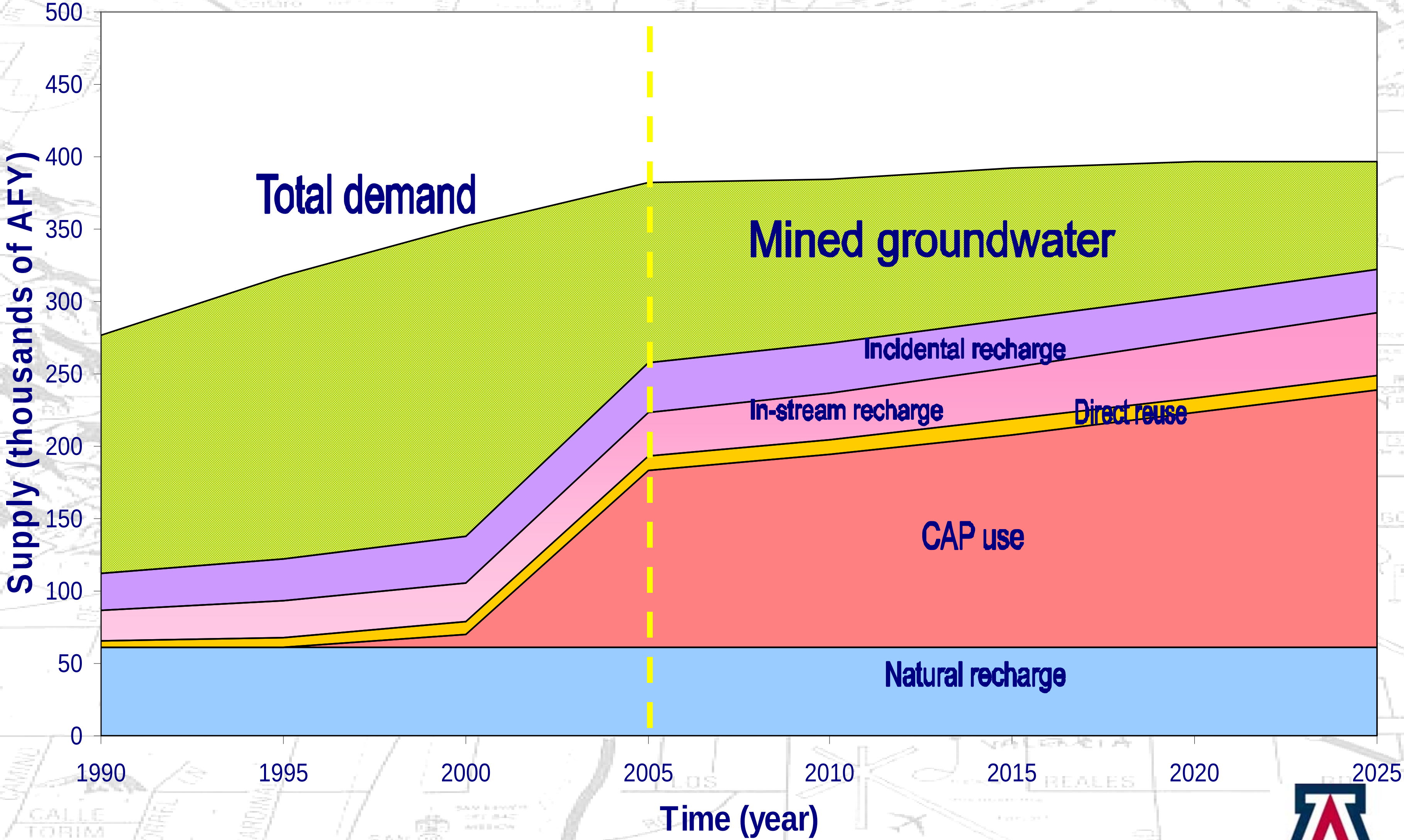


Total demand is 380,000 AFY

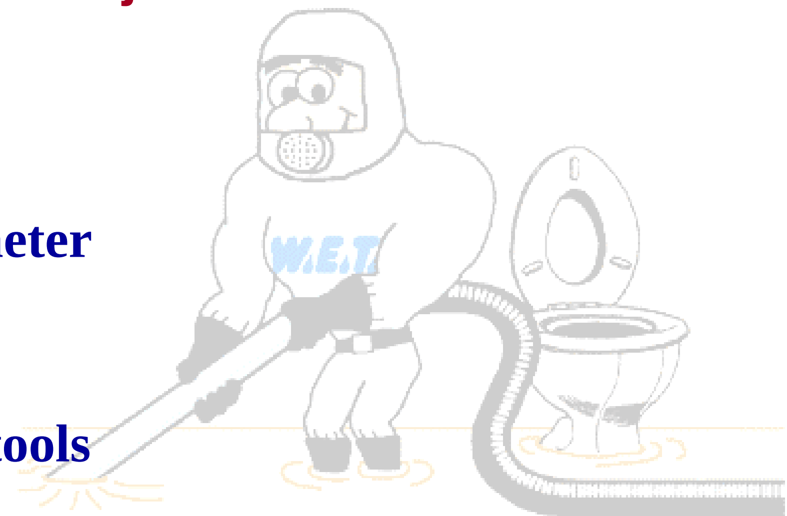
Water Supply by Source (2005)



Water Supply and Demand in the Tucson Active Management Area



The Overall Goal of the Project



- Include water quality as a modeled parameter
  - ➢ Create new water sources by reuse
- Build up comprehensive and educational tools
  - ➢ Mathematically represent the physical system and consider all major water sources
  - ➢ Improve water resources management decisions
  - ➢ Predict future water conditions

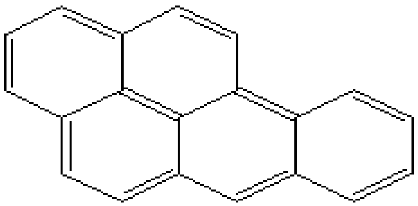
The Main Classes of Contaminants

- Biochemical Oxygen Demand (BOD)
- Total Dissolved Solids (TDS)
- Total Suspended Solids (TSS)
- Total Organic Carbon (TOC)
- Hardness
- Total Nitrogen
- Total Phosphorus
- Total Coliform

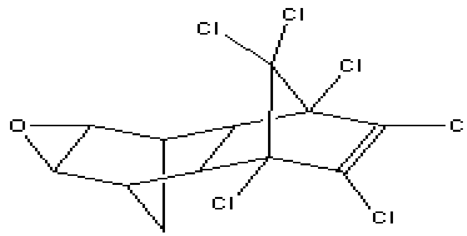
Additional Specific Contaminants Considered

Carcinogens

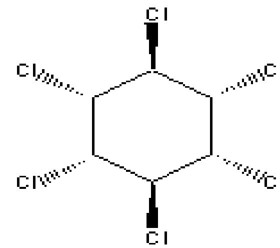
Benzo[a]pyrene



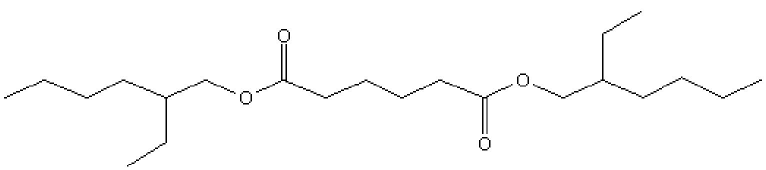
Dieldrin



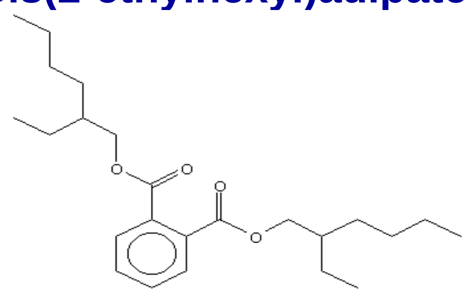
Lindane*



Bis(2-ethylhexyl)phthalate



Bis(2-ethylhexyl)adipate

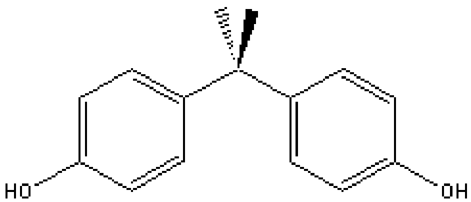


*** No carcinogenicity assessment exist but it is in the list due to HQ number (toxicity)**

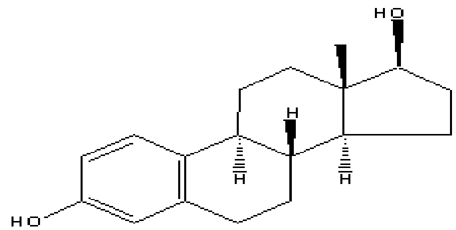
Additional Specific Contaminants Considered

Endocrine Disruptor Compounds

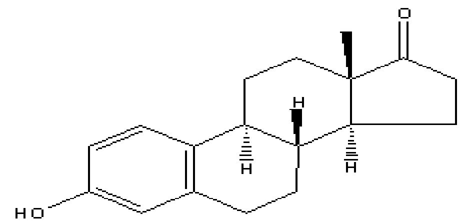
Bisphenol A



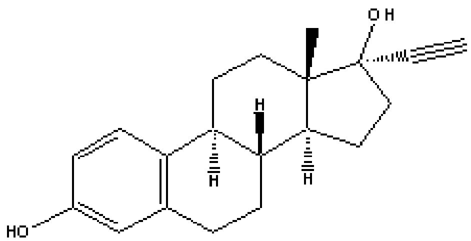
β-estradiol (E2)



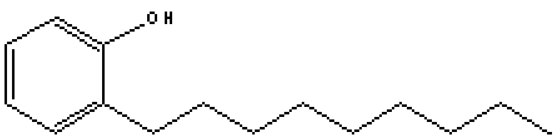
Estrone



Ethynyl estradiol (EE2)



Nonylphenol (NP)

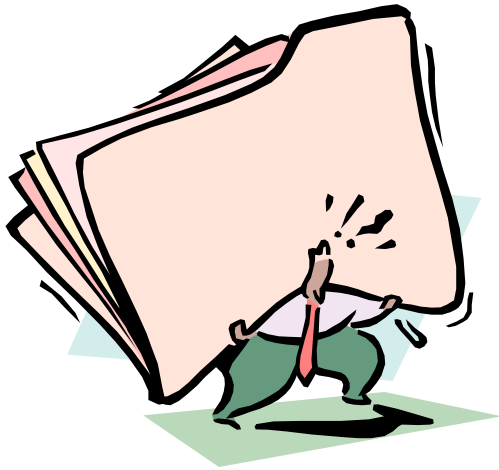


Heavy Metals

Arsenic (As) | **Mercury (Hg)** | **Lead (Pb)**

Choice of Specific Contaminants

Why these compounds?



- **US EPA Integrated Risk Information System (IRIS)**
  - **listed as probable human carcinogens**

- **US Geological Survey the first nationwide reconnaissance of the occurrence of pharmaceuticals, hormones, and other organic wastewater contaminants (OWCs) in water resources (D. W. Kolpin, *et al*, 2002)**
  - **risk assessment analysis**

Risk Assessment Analysis

"the characterization of the potential adverse health effects of human exposures to environmental hazards" (NRC, 1983)

Hazard Quotient: Non-carcinogenic (toxicity) effect

$$HQ = \frac{C_i \times ADWI}{ABW} \times \frac{1}{RfD}$$

- **C_i : concentration of the contaminant (mg/l)**
- **RfD : reference dose for chronic oral exposure (mg/kg-d)**
- **For an adult**
  - ➢ **ADWI : average daily water intake = 2 l/d**
  - ➢ **ABW : average body weight = 70 kg**

Risk Assessment Analysis

"the characterization of the potential adverse health effects of human exposures to environmental hazards" (NRC, 1983)

Risk: The probability of adverse effects resulting from exposure to an environmental agent or mixture of agents (level of carcinogenicity)

$$\text{Risk} = \frac{C_i \times \text{ADWI}}{\text{ABW}} \times \text{Oral PF}$$

- **C_i : concentration of the contaminant (mg/l)**
- **Oral PF : oral potency factor $(\text{mg/kg-d})^{-1}$**
- **For an adult**
  - **ADWI : average daily water intake = 2 l/d**
  - **ABW : average body weight = 70 kg**

Risk Assessment Analysis

A brief summary of the contaminants chosen

Name of the Contaminant	Oral Intake		Carcinogenicity	
	RfD	HQ	Oral PF	Risk
	(mg/kg-day)	(-)	(mg/kg-day)-1	(-)
Benzo[a]pyrene	-	-	7.30E+00	5.01E-05
Bis(2-ethylhexyl)adipate	6.00E-01	4.76E-04	1.20E-03	3.43E-07
Bis(2-ethylhexyl)phthalate	2.00E-02	2.86E-02	1.40E-02	8.00E-06
Bisphenol A	5.00E-02	6.86E-03	-	-
Dieldrin	5.00E-05	1.20E-01	1.60E+01	9.60E-05
Lindane	3.00E-04	1.05E-02	-	-
β-estradiol (E2)	-	-	-	-
Ethynyl estradiol (EE2)	-	-	-	-
Nonylphenol (NP)	-	-	-	-
Estrone	-	-	-	-
Arsenic	3.00E-04	-	1.50E+00	-
Lead	In discussion	-	reas. anticip.	-
Mercury	NA	-	inadequate	-

Physical & Chemical Properties of Importance in Design

- MW (molecular weight)
- Density
- Melting Point
- Boiling Point
- Water Solubility
- Henry's Constant
- K_{OC} (organic-carbon partition coefficient)
- K_{OW} (octanol-water partition coefficient)
- Freundlich Parameters (K & 1/n)
- Degradation Coefficient
- Vapor Pressure

How to Obtain?

Data sources:

- **Reference and text books**

  Merck Index, Water Quality and Treatment (AWWA), etc.

- **World-Wide Web**

  NIST Chemistry WebBook, Chemfinder, etc.

- **Estimation methods**

  Group Contribution Methods, e.g. Joback Method

Estimation of Unknown Properties

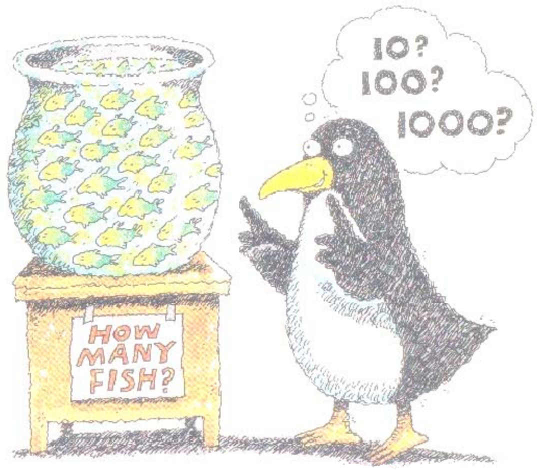
Joback's Group Contribution Estimation Method:

- **Boiling Point** $T_b(K) = 198 + T_{b1} + T_{b2} + T_{b3} + ...$
- **Melting Point** $T_f(K) = 122 + T_{f1} + T_{f2} + T_{f3} + ...$
- **Critical Temperature** $T_c(K) = T_b / (0.584 + 0.965\ S - S^2)$
- **Critical Pressure** $P_c(bar) = 1 / (0.113 + 0.0032\ n - S)^2$

Liquid Density Prediction:

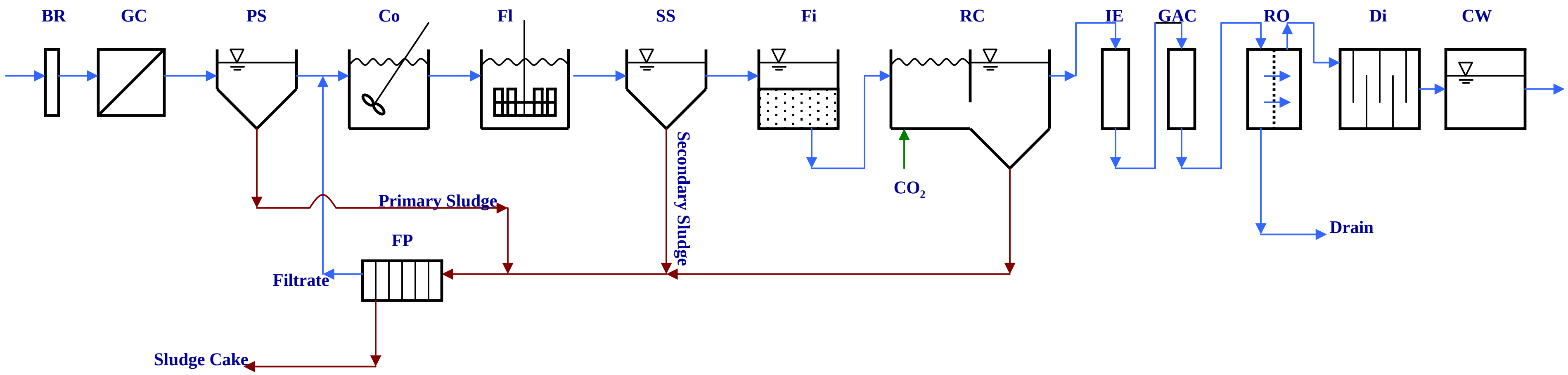
$$\frac{1}{\rho_{sat}} = V_{sat} = \left(\frac{R \times T_C}{P_C}\right) \times Z_{RA}^{n}$$

$$n = 1.0 + (1.0 - T_r)^{2/7}$$



Z_{RA}^{n} :critical compressibility factor (-)
T_r :reduced temperature (K)
R :gas constant (8.3140 m³ kPa/kmole K)

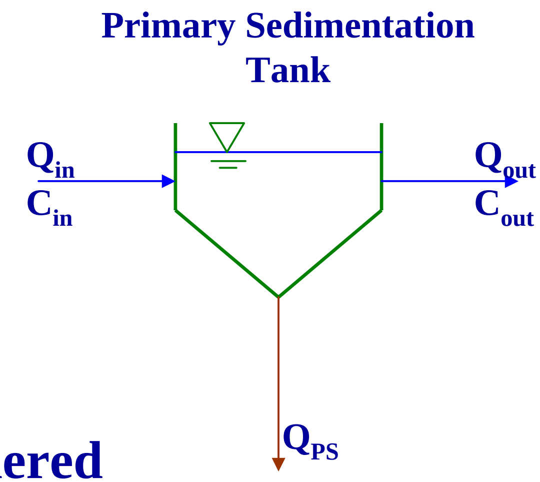
Water Treatment Unit Operations Train

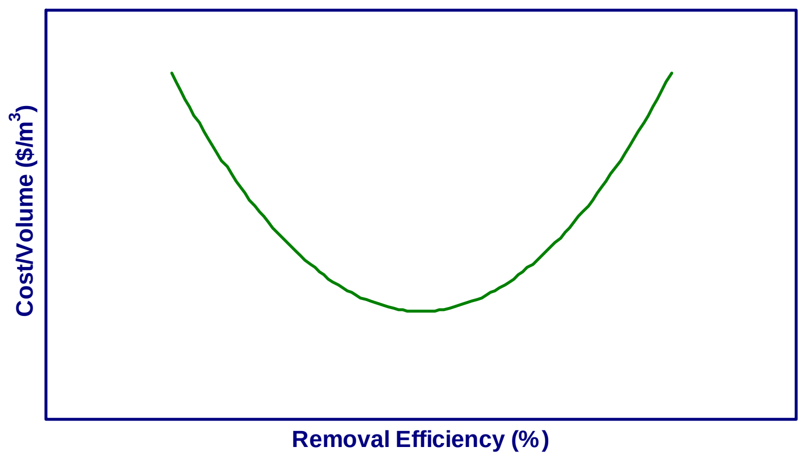


BR: Bar rack
GC: Grit Chamber
PS: Primary Sedimentation
Co: Coagulation
Fl: Flocculation
SS: Secondary Sedimentation
Fi: Filtration
RC: Recarbonation
IE: Ion Exchange
GAC: Granular Activated Carbon
RO: Reverse Osmosis
Di: Disinfection
CW: Clear Well
FP: Filter Press

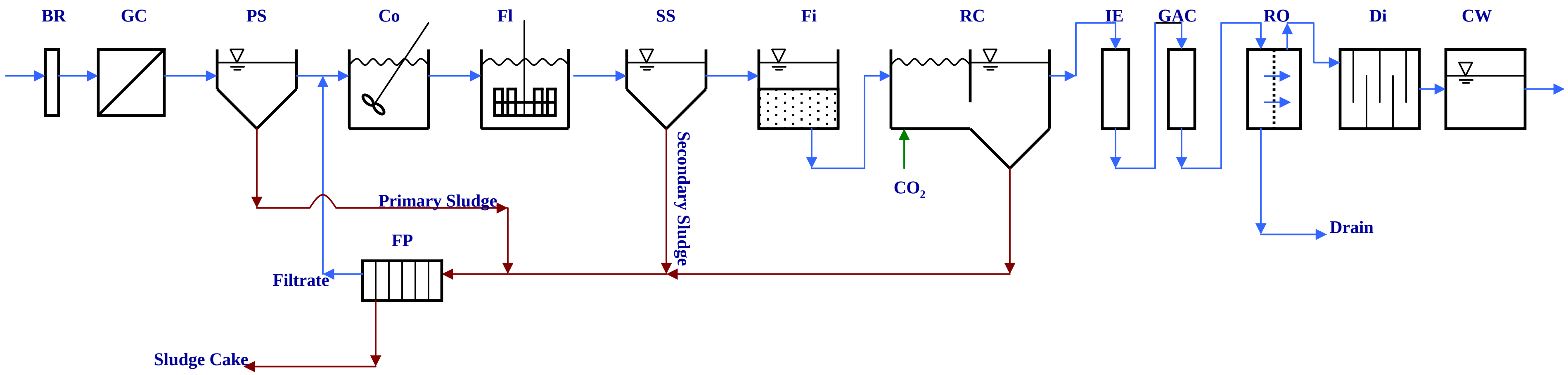
Primary Sedimentation Basin as a Unit Operation

- random number assigned by the program (0-100)
- defines:
  - volume of the PS basin
  - dimensions of the basin ➡ # of PS units
  - removal efficiency for each contaminant considered
- keep the cost to a minimum





Optimization of the Treatment Plant



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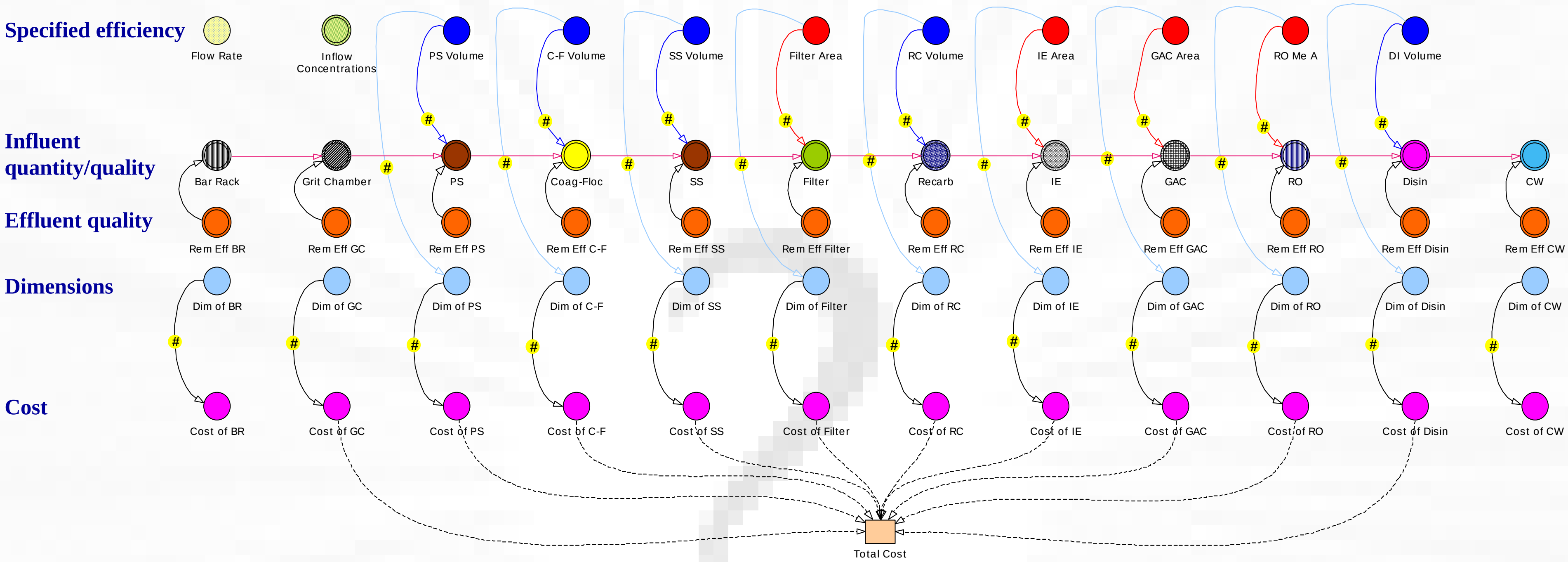
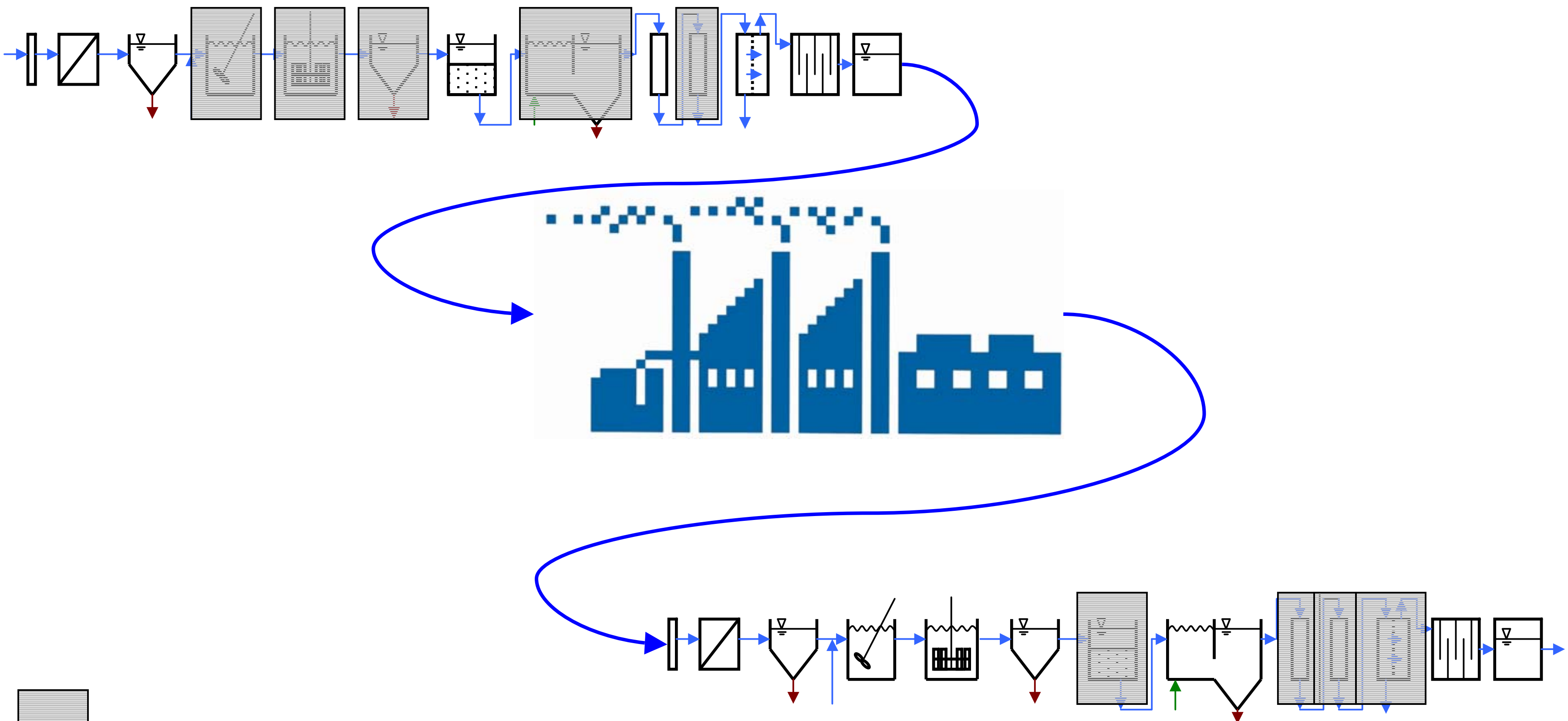


How it works?

- the unit volume/area assigned by the program
- calculate the efficiency of the specific unit operation
- calculate the dimensions/# of the specific unit operation
- calculate the cost/total cost

Optimization of the Treatment Plant

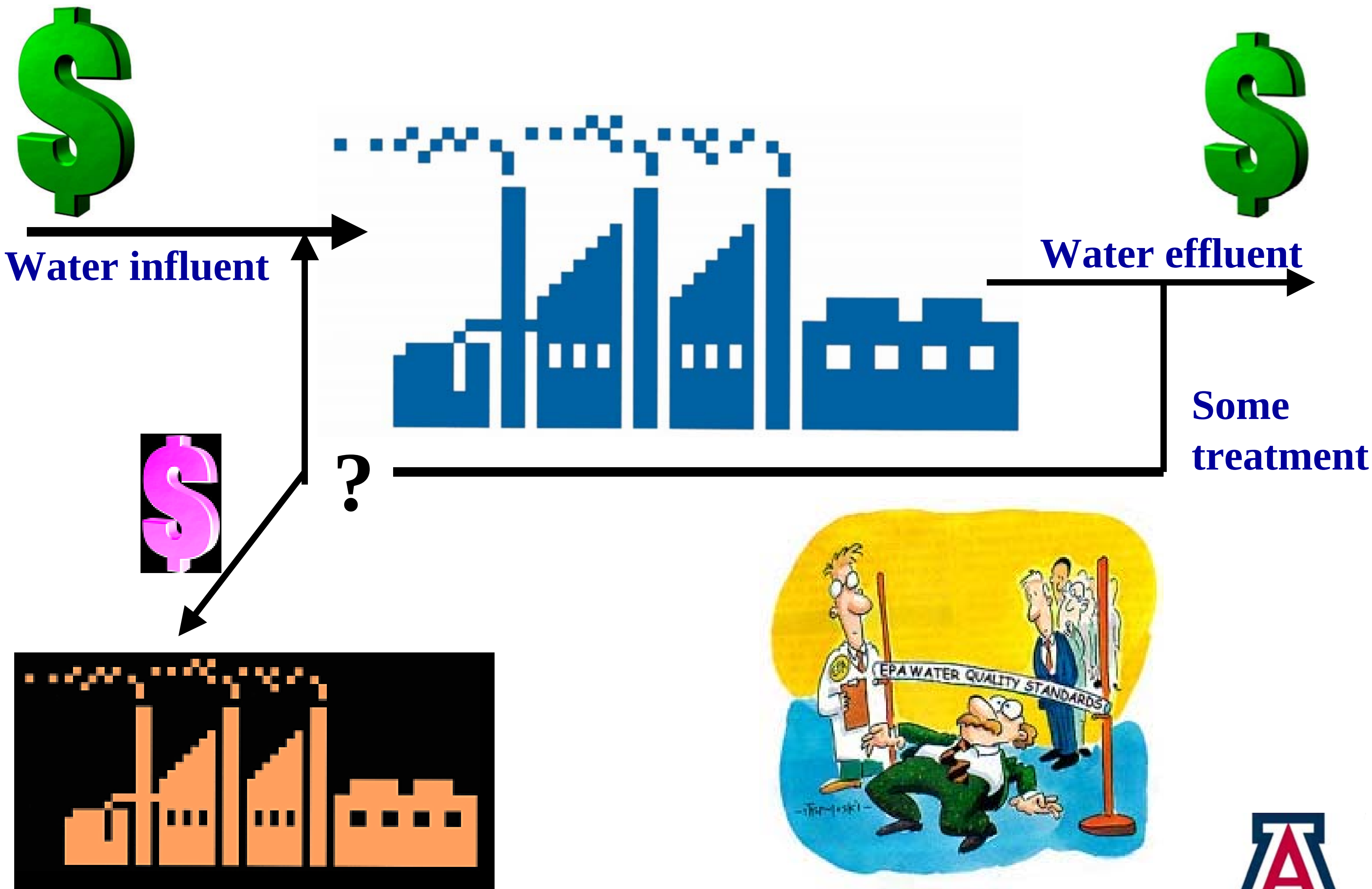
Pre-treatment Unit Operations Train



“turned off” unit operations

Post-treatment Unit Operations Train

As a Result


Water influent
Water effluent
?
Some
treatment
EPA WATER QUALITY STANDARDS

As a Result

- **Socially- if more industrial companies use this kind of recycled water, we are going to have a positive influence on public perception and improve company image**
- **Economically- industry will have opportunity to save money and energy**
- **Environmentally- it is very efficient to reuse water with the minimum treatment**

Therefore, here we will benefit from three major aspects. It will be a win-win situation for industry, even the whole society.

Acknowledgements

- NSF/SRC ERC for Environmentally Benign Semiconductor Manufacturing
  - ➢Special thanks to Dr. Shadman and Dr. Ogden at UofA ERC
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- The entire modeling team lead by Dr. Lansey
- SAHRA (Sustainability of semi-Arid Hydrology and Riparian Areas)
- Southern Arizona Water Users Association
- Upper San Pedro Partnership
- Nature Conservancy
- ERC industrial members (Motorola, Pall Corporation, and Texas Instruments)
- Sandia National Laboratory (SNL)