Summary of Activities and Next Steps
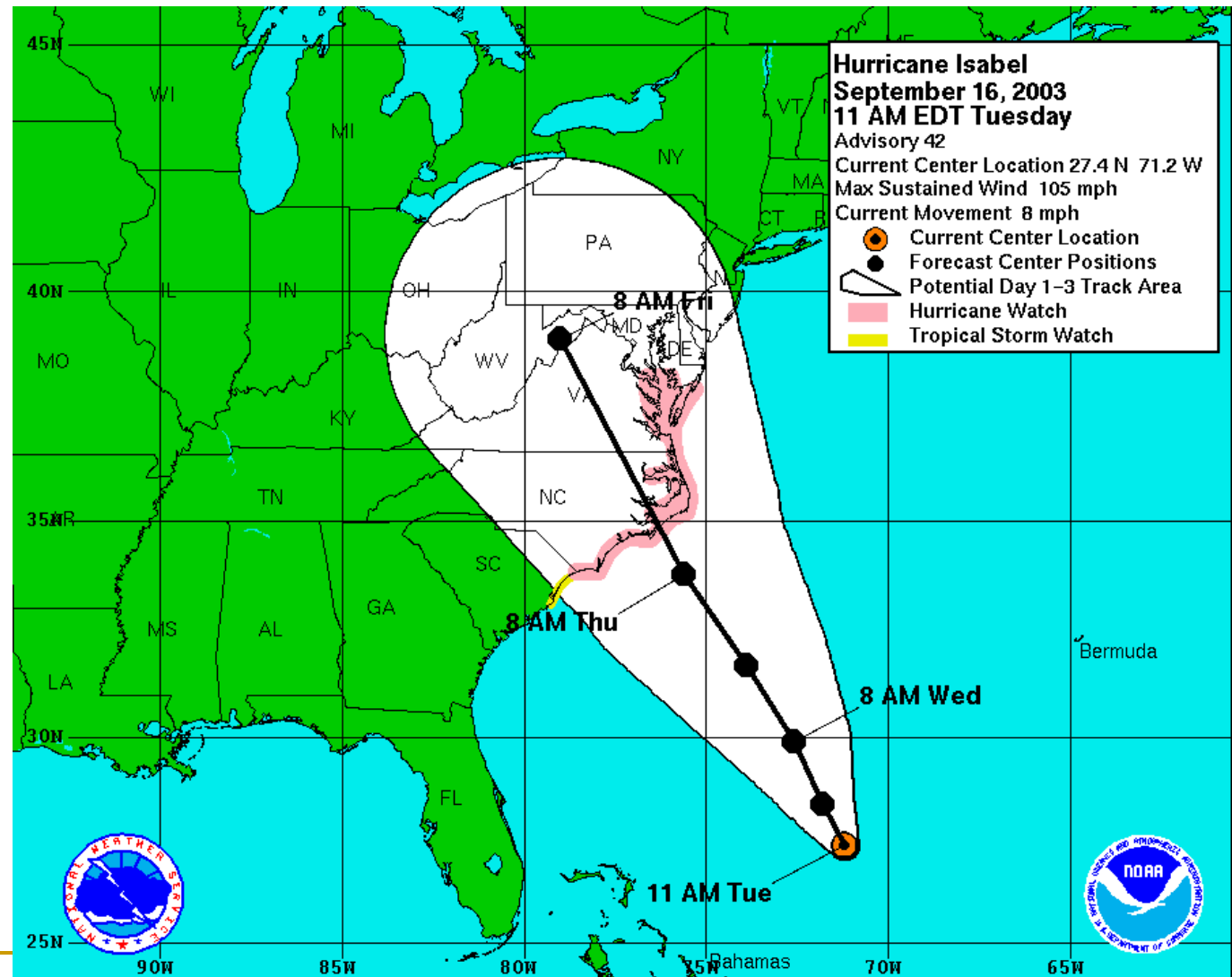
Report for the NDWAC CCL Work Group

September 17, 2003

Overview

- We've made significant progress on the universe and types of data needed

- We've made progress on steps that need to be tackled in series -- screening tools, attribute scoring , surrogate data

- We need to finalize some discussion points and we are close

- Today's discussion will focus on what we've done, where we are, what we need to do
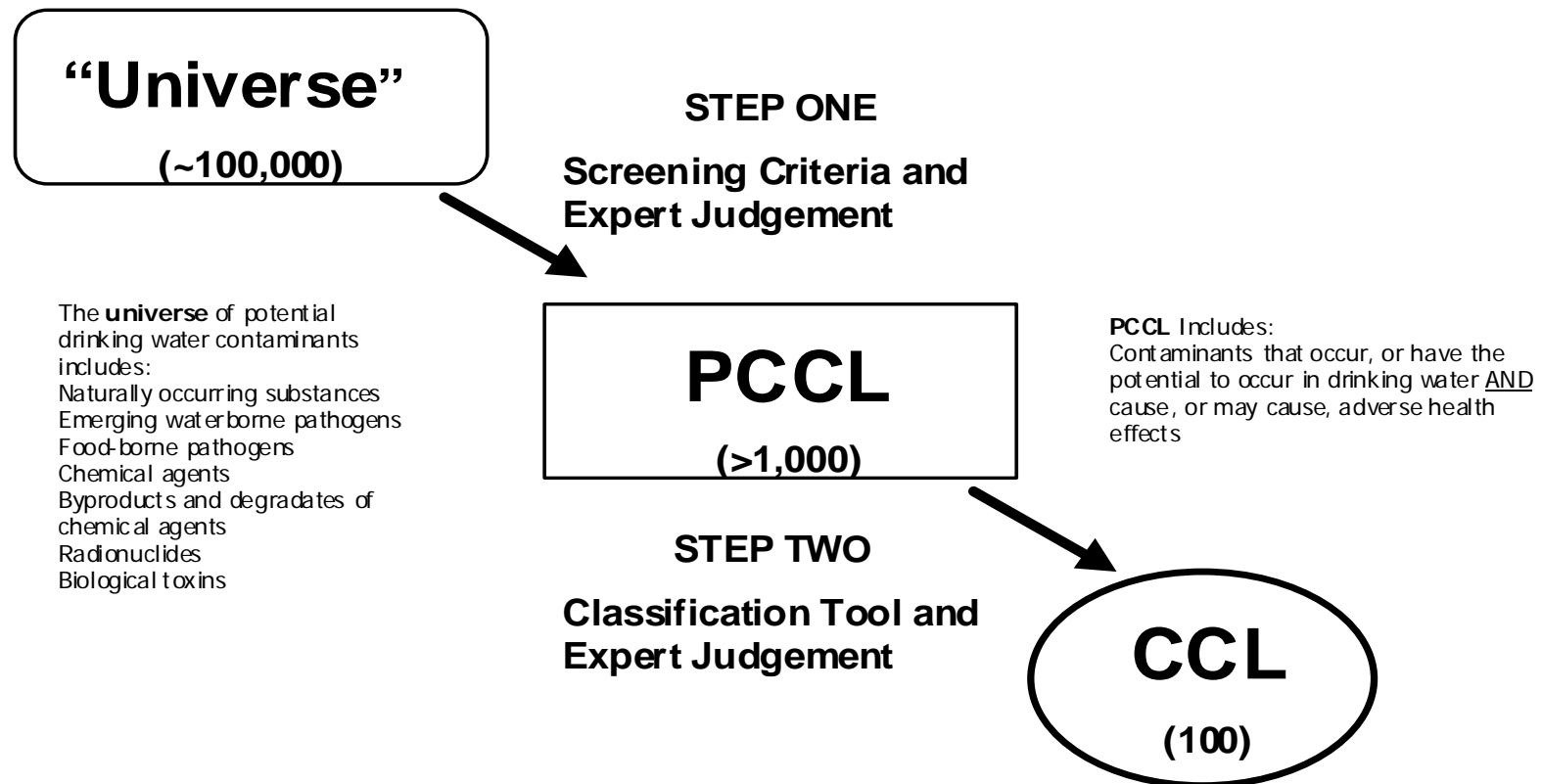
Isabel Update

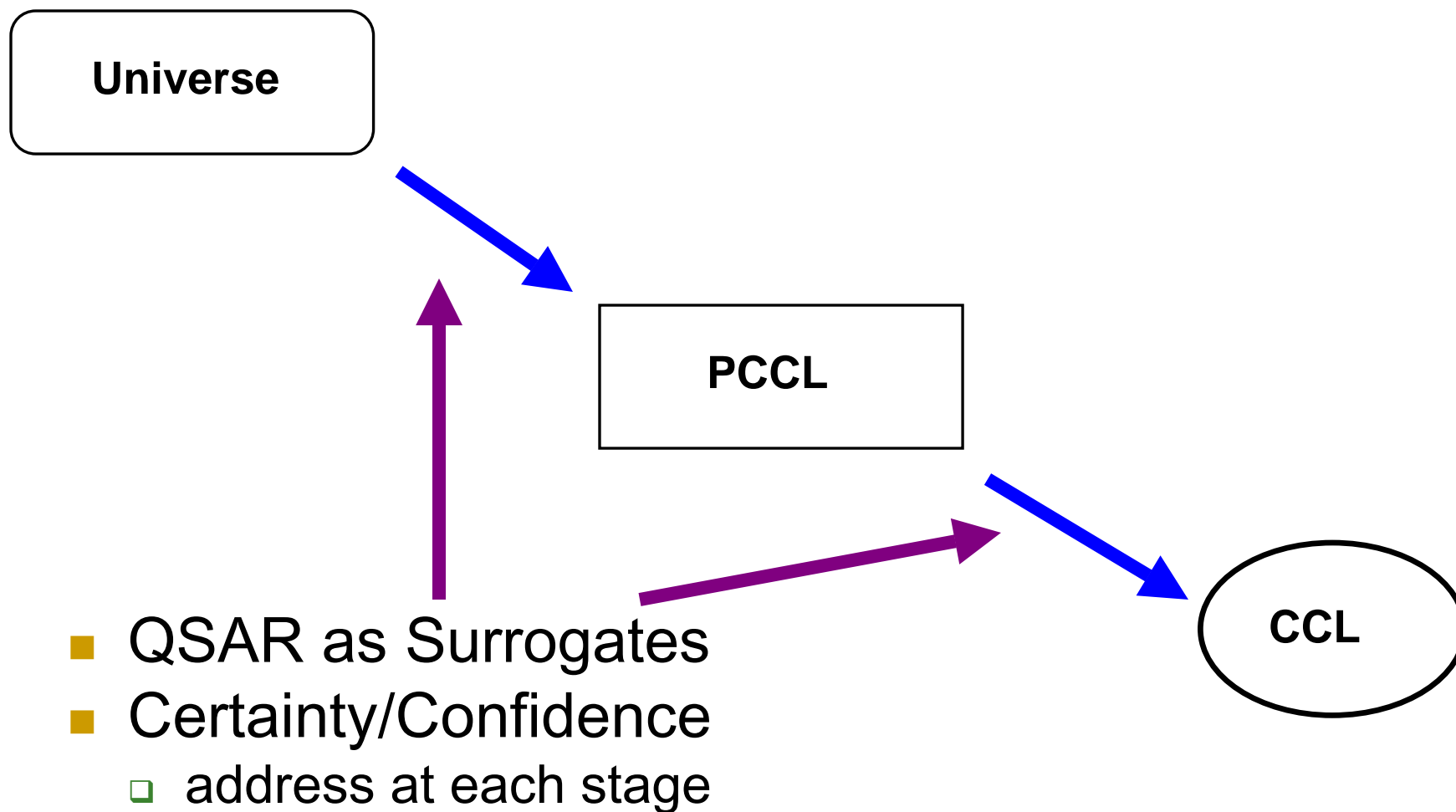**"We operate out of flexibility, not confusion"**

THANK YOU

Overview

NRC Recommendations for the CCL

"Universe"

(~100,000)

STEP ONE

Screening Criteria and Expert Judgement

The **universe** of potential drinking water contaminants includes:
Naturally occurring substances
Emerging waterborne pathogens
Food-borne pathogens
Chemical agents
Byproducts and degradates of chemical agents
Radionuclides
Biological toxins

PCCL

(>1,000)

PCCL Includes:
Contaminants that occur, or have the potential to occur in drinking water <u>AND</u> cause, or may cause, adverse health effects

STEP TWO

Classification Tool and Expert Judgement

CCL

(100)

Critical path decisions

Universe

PCCL

CCL

- QSAR as Surrogates
- Certainty/Confidence
  - address at each stage

Universe -- Progress Made

- Identified over 200 data sources

- Evaluating those data sources based on Work Group Guidance and principles

- Developed an example data set that is representative of a CCL universe.

- Microbial universe developed on available literature and consistent with chemical Universe

Universe -- Next Steps

- NDWAC guidance has given us a good roadmap for the universe

- Technical team to complete characterization of the data sources considered

- Evaluate technical options for data extraction
- analyses, and document the CCL decisions

- Complete Chapter 5 of Report

Universe to PCCL -- Progress Made

- Developed the Gate concept

- Performed preliminary analyses on types of data and how the data align at the gates

- Qualitative and Quantitative approaches tested on Example data set

- Concepts are discussed in chapter 6

Universe to PCCL -- Progress made

- Work Group requested additional analyses
  - Surrogate information available
    - QSARs developed for ~700 chemicals
    - QSARs can predict toxicity and solubility and biodegradation information
    - QSAR will not work on all chemicals, ~50% in sample exercise had model errors for health effects
    - TopKat was the QSAR model used

  - Binning approach for screening
    - Preliminary work was started
    - Used chemicals from example data set and QSAR analyses
    - Binning seems to be straightforward approach and is consistent with NRC and subsequent steps (attributes)

Universe to PCCL -- Next steps

- Evaluate utility of QSAR and surrogate data

- Evaluate binning analyses as an effective screening tool

- Discuss the data sources and data elements needed for screening, we've got start on this

- Micro Subgroup is working on a set of criteria to develop PCCL from Universe of microbial contaminants

PCCL to CCL -- Progress made

- Began discussion on Models, Certainty, and Attributes

- Steps discussed theoretically

- 5 attributes capture the right characteristics

- We identified on the types of data we'll need

PCCL to CCL -- Models

- **Classification models presentation**
  - Reviews the classification process
  - Addresses what the models can accomplish
  - Issue: Are we trying to apply a precision beyond what the models can achieve

- **Certainty and Confidence**
  - Presentation of issues and options

PCCL to CCL -- Attributes

- Developed a set of data to test attributes scoring
  - 40 chemicals from 17 data sources
  - Extracted and organized data from text and bibliographic sources
- Learned some lessons in developing the scoring rules
  - Potency and Prevalence can use scoring based on the range of data
  - Scoring across types of data can be consistent
  - Severity and Microbial attribute scoring requires experts and may not be amenable to automation

PCCL to CCL -- Attributes

- **Severity Scoring**
  - Can we overcome subjectivity in scoring
  - Does reducing the scoring scale help reduce the subjectivity

- **Preliminary work started on Persistence & Mobility**

- **Preliminary work started on Magnitude**
  - Builds on Potency and Prevalence

PCCL to CCL -- Next Steps

- How can we incorporate surrogates into the attribute scoring
    - Results from the QSAR presentation
    - Results from the Potency discussion

- Calibration and reproducibility are discussed in the potency and prevalence presentations
    - Consistency across types of data
    - Consistency between CCLs

- Is Persistence and Mobility a surrogate for Prevalence or a separate attribute

PCCL to CCL -- Next Steps

- Need to complete the attribute discussion to test the classification models

- Transparency and reproducibility of classification models must be evaluated

Onward, upward, together

- Universe to PCCL to CCL

- Agree on progress made?

- Agree on Next Steps?

- What did we miss?