
Summary of Activities and Next Steps

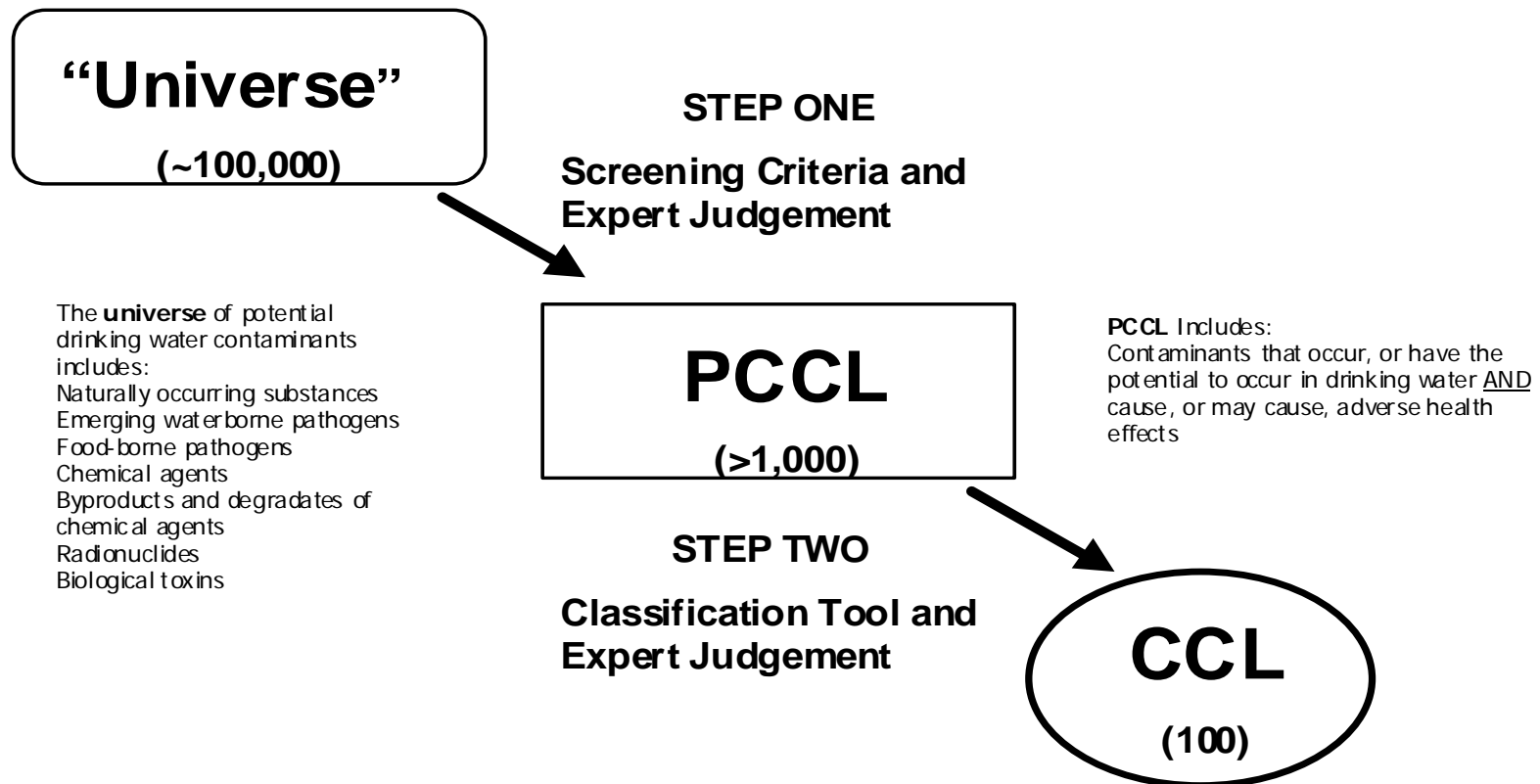
Report for the NDWAC CCL Work Group
September 17, 2003

Overview

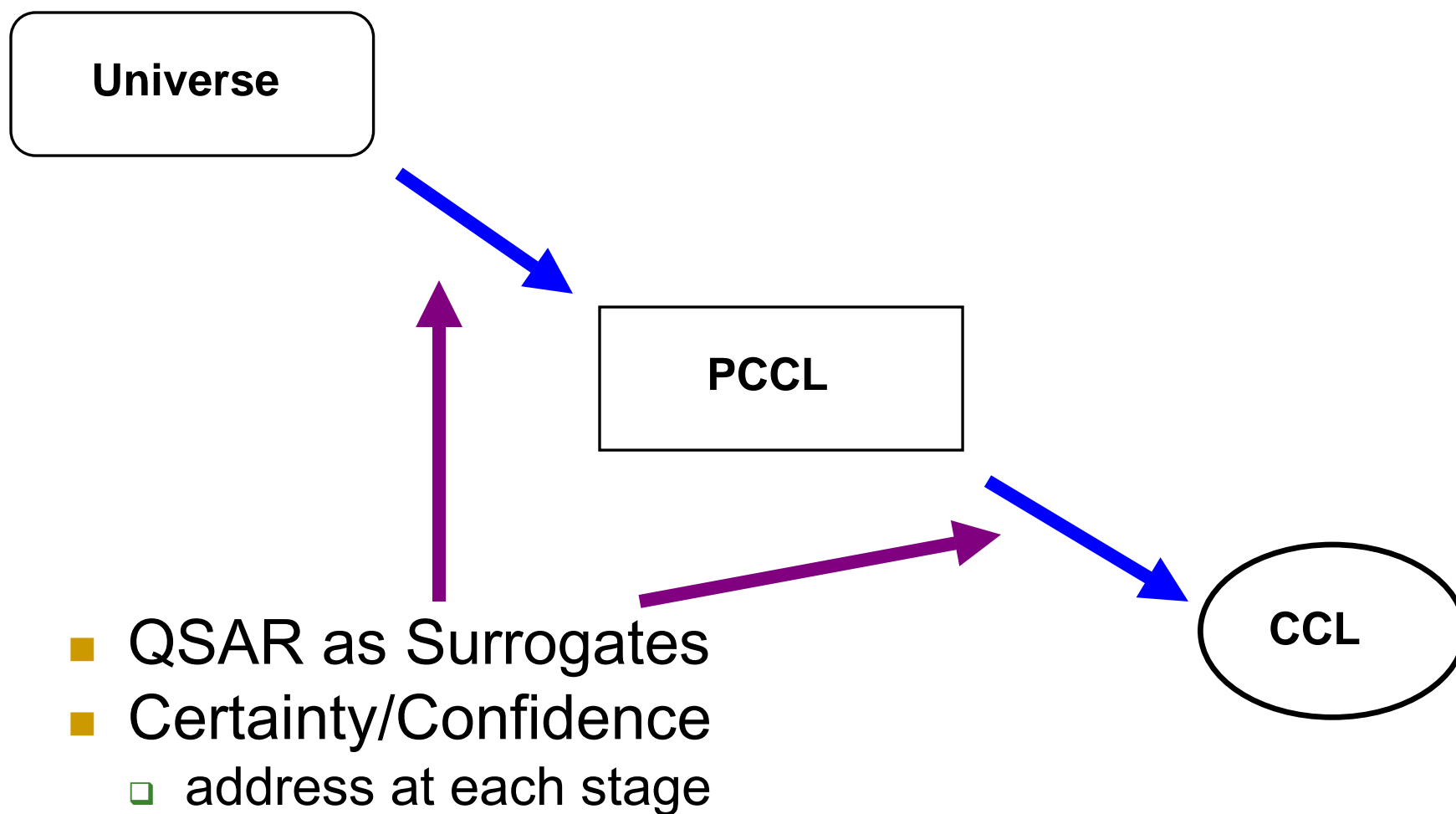
- We've made significant progress on the universe and types of data needed
- We've made progress on steps that need to be tackled in series -- screening tools, attribute scoring , surrogate data
- We need to finalize some discussion points and we are close
- Today's discussion will focus on what we've done, where we are, what we need to do

Overview

NRC Recommendations for the CCL



Critical path decisions



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
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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?