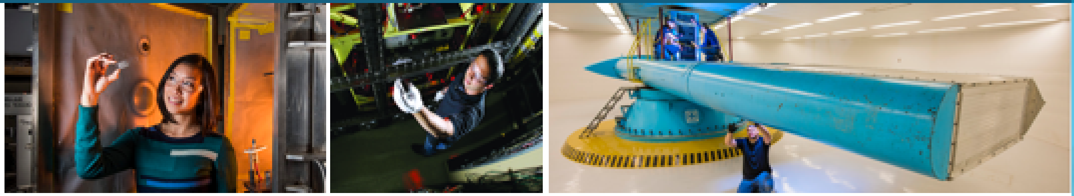
SAND2021-12958PE

MACCS Initiatives for Advanced Reactor Consequence Analyses



PRESENTED BY

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Full Radionuclide Screening report prepared by Nathan Andrews, Michael Higgins, Anna Taconi, and Jennifer Leute

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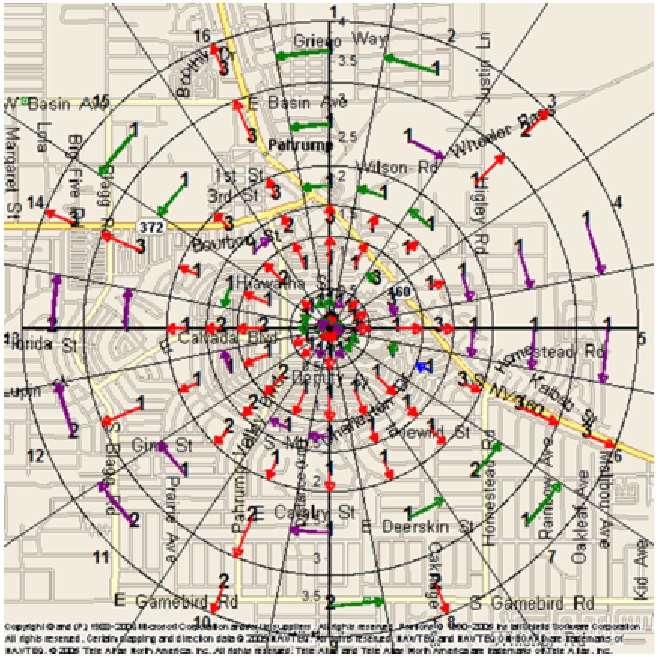
Contents

- What is MACCS and what is it used for?
- Advanced reactor initiatives
- Radionuclide screening:
    - Background
    - MACCS Capabilities
    - Approach
    - High Temperature Gas Reactors (HTGRs)
    - Molten Salt Reactors (MSRs)
    - Fluoride Salt Cooled High Temperature Reactors (FHRs)
    - Liquid Metal Reactors (LMRs)
    - Follow-on activities

What is MACCS and what is it used for?

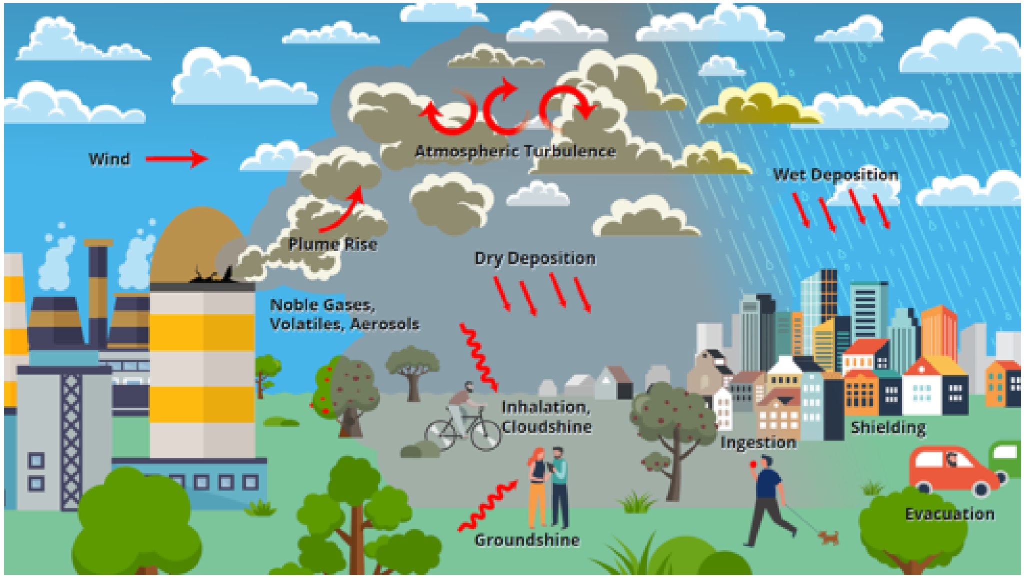
- Nuclear accident consequence analysis code
- Simulates the release of radioactive material on the surrounding environment
- Calculates concentrations, health effects, and economic consequences
- Uses include:
  - Nuclear facility licensing
  - Emergency planning and response
  - Probabilistic Risk Assessments (PRA)



MACCS Network Evacuation Map

Phenomena Treated by MACCS

- Representation of source term
- Atmospheric transport and dispersion
  - Statistical sampling of archived weather data
- Wet and dry deposition
- Exposure pathways to humans
  - Inhalation
  - Cloudshine
  - Groundshine
  - Resuspension
  - Ingestion



- Emergency actions
  - Sheltering
  - Evacuation
  - KI ingestion
  - Relocation
- Long-term remedial actions
  - Decontamination
  - Temporary or permanent interdiction of property
  - Crop disposal
- Economic losses
  - Evacuation and relocation per diem costs
  - Long-term relocation cost
  - Decontamination costs
  - Loss of property use
  - Depreciation during interdiction
  - Property value for permanent interdiction

How might advanced reactors be different?

- PWR
- BWR

GEN II

- AP1000
- ESBWR

GEN III +

- NuScale
- B&W mPower
- Holtec SMR-160
- Westinghouse SMR

SMR

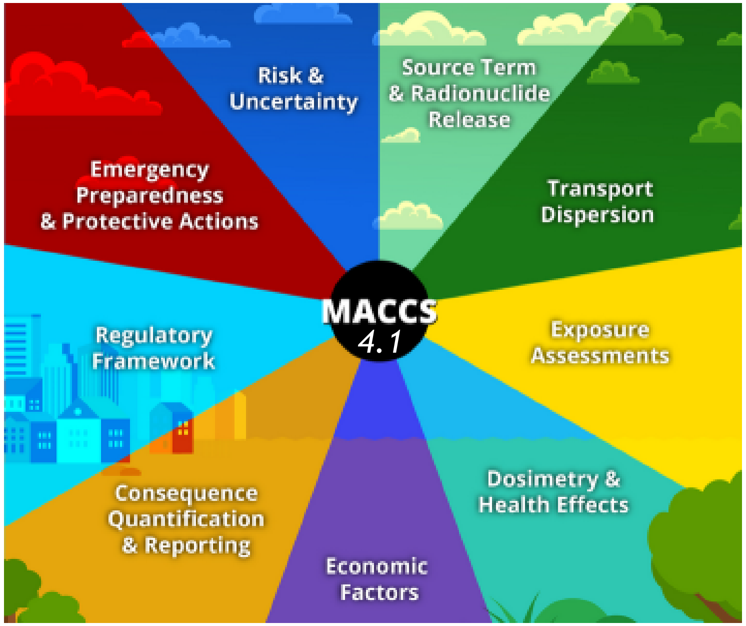
- Sodium Fast Reactor
- High Temperature Gas Reactor
- Lead Fast Reactor
- Gas Fast Reactor
- Molten Salt Reactor

GEN IV Advanced Reactors

- Significant differences in design, size, spectrum, and materials
- Different reactor materials lead to differences in activation products
- Different fuels lead to differences in fission products and actinides
- All of these aspects lead to changes in releases and associated health and economic consequences following an accident

Advanced Reactor Initiatives

- Modeling near-field dispersion
  - Release of MACCS 4.1
  - Potential update for HYSPLIT
- Radionuclide screening
  - Preliminary assessment of potentially released radionuclides from HTGRs, MSRs, FHRs, and LMRs
  - Next step to evaluate gaps and priorities for consequence analysis
- MelMACCS update in process:
  - Expansion of inventories
  - More flexibility in chemical group selection



MACCS 4.1 was released on 30 July 2021

Radionuclide Screening - Background

- Currently a set of 71 radionuclides are accounted for in off-site consequence analysis for light water reactors (LWRs)
- Radionuclides of dose consequence are expected to change for non-LWRs, with radionuclides of interest being reactor type-specific
- SAND2021-11703 provides a preliminary and expanded set of radionuclides that may need to be accounted for in multiple non-LWR systems:
    - high temperature gas reactors (HTGRs)
    - fluoride-salt-cooled high-temperature reactors (FHRs)
    - thermal-spectrum fluoride-based molten salt reactors (MSRs)
    - fast-spectrum chloride-based MSRs
    - liquid metal fast reactors with metallic fuel (LMRs)

MACCS Capabilities

- There are 825 radionuclides that can be currently selected in MACCS
- Up to 150 radionuclides can be selected at a time
- The 71 radionuclides typically used for LWRs are grouped into 10 chemical groups
    - *Relative Importance of Individual Elements to Reactor Accident Consequences Assuming Equal Release Fractions [2]*
    - SOARCA

Chemical Group	Isotope	Half-life	Chemical Group	Isotope	Half-life
Noble Gas	Kr-85	10.72 yr	Early Transition Elements	Co-58	70.8 d
	Kr-85m	4.48 hr		Co-60	5.271 yr
	Kr-87	76.3 min		Nb-95	35.1 d
	Kr-88	2.84 hr		Nb-97	72.1 min
	Xe-133	5.25 d		Nb-97m	1.0 min
	Xe-135	9.09 hr		Mo-99	66.0 hr
	Xe-135m	15.3 min		Tc-99m	6.02 hr
Alkali Metals	Rb-86	18.7 d	Tetravalents	Zr-95	64.0 d
	Rb-88	17.8 min		Zr-97	16.9 hr
	Cs-134	2.062 yr		Ce-141	32.5 d
	Cs-136	13.1 d		Ce-143	33.0 hr
	Cs-137	30.0 yr		Ce-144	284.3 d
Alkaline Earths	Sr-89	50.5 d		Np-239	2.35 d
	Sr-90	29.1 yr		Pu-238	87.74 yr
	Sr-91	9.5 hr		Pu-239	2.41E4 yr
	Sr-92	2.71 hr		Pu-240	6.54E3 yr
	Ba-137m	2.55 min		Pu-241	14.4 yr
	Ba-139	82.7 min	Trivalents	Y-90	64.0 d
	Ba-140	12.74 d		Y-91	58.5 d
Halogens	I-131	8.04 d		Y-91m	49.7 min
	I-132	2.30 hr		Y-92	3.54 hr
	I-133	20.8 hr		Y-93	10.1 hr
	I-134	52.6 min		La-140	40.3 hr
	I-135	6.61 hr		La-141	3.9 hr
Chalcogens	Te-127	9.35 hr		La-142	92.5 min
	Te-127m	109 d		Pr-143	13.56 d
	Te-129	69.6 min		Pr-144	17.3 min
	Te-129m	33.6 d		Pr-144m	7.2 min
	Te-131	25.0 min		Nd-147	11.0 d
	Te-131m	30.0 hr		Am-241	432.2 y
	Te-132	78.2 hr		Cm-242	162.8 d
Platinoids	Ru-103	39.3 d		Cm-244	18.11 yr
	Ru-105	4.44 hr	Cadmium Group	Sb-127	3.85 d
	Ru-106	368.2 d		Sb-129	4.32 hr
	Rh-103m	56.1 min			
	Rh-105	35.4 hr			
	Rh-106	29.9 sec			

Approach

Examine reactor design and inventory*

Evaluate potential chemical forms

Evaluate potential release amounts

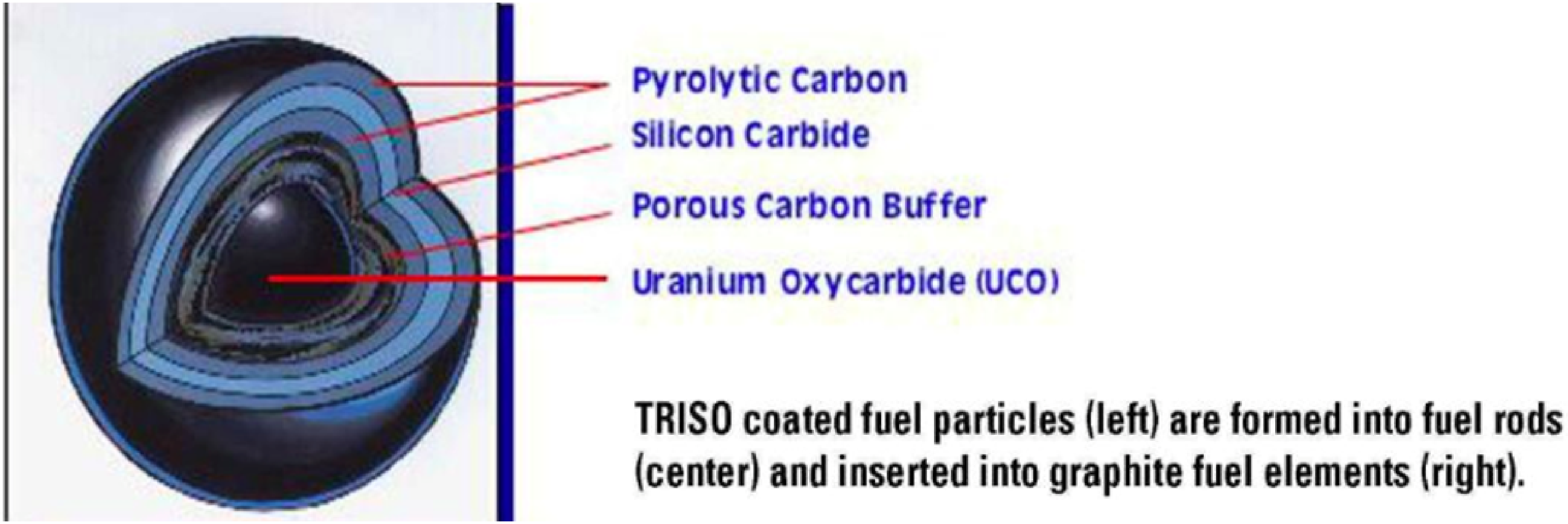
Screen based on sufficient quantities and radiotoxicity

Assign to current chemical groups, or propose new ones

*This analysis based on best available inventory data

High Temperature Gas Reactors

- TRi-structural ISOtropic (TRISO) fuel
- U-235 as the primary fissile material
- Thermal spectrum
- Inert gas coolant



TRISO coated fuel particles (left) are formed into fuel rods (center) and inserted into graphite fuel elements (right).

TRISO Fuel Structure [6]

HTGR Radionuclides of Interest

Element	Isotope	Corresponding Chemical Group
H	3	Proposed New Group
C	14	Proposed New Group
Ag	110m	Tin Group
Sb	125	Cadmium Group
Pm	147	Trivalents
Sm	151	Trivalents
Eu	154	Trivalents
	155	
Pu	242	Tetravalents
Cm	244	Trivalents
	245	

Molten Salt Reactors

- Thorium, uranium or plutonium-based fuel dissolved in a fluoride or chloride-based salt
- Fluoride-based systems will be fueled with either a Th-232/U-233 thermal-spectrum breeder salt or a U-235/U-238 thermal-spectrum salt
- Chloride-based systems would likely be fueled with a combination of a U-235/U-238/Pu-239 and operate in a fast spectrum
- Gaps exist in the design, materials and neutronics
- Molten Salt Reactor Experiment (MSRE) data was used and an evaluation of cumulative fission yields of U-233, U-235, and Pu-239

Fluoride Salt Thermal Spectrum-1

Nuclide	Corresponding Chemical Group	Nuclide	Corresponding Chemical Group
H-3	Proposed New Group	Sb-128	Cadmium Group
Na-22	Alkali Metal	Te-125m	Chalcogens
Na-24	Alkali Metal	Te-133m	Chalcogens
As-77	Cadmium Group	Te-134	Chalcogens
Se-81	Chalcogens	Xe-131m	Noble Gas
Se-81m	Chalcogens	Xe-133m	Noble Gas
Se-83	Chalcogens	Pr-146	Trivalents
Br-83	Halogen	Pm-147	Trivalents
Br-84	Halogen	Pm-148m	Trivalents
Kr-83m	Noble Gas	Pm-149	Trivalents
Nb-93m	Trivalents	Pm-151	Trivalents
Pd-109	Platinoids	Sm-151	Trivalents

Fluoride Salt Thermal Spectrum-2

Nuclide	Corresponding Chemical Group	Nuclide	Corresponding Chemical Group
Pd-112	Platinoids	Sm-153	Trivalents
Ag-111	Tin Group	Eu-154	Trivalents
Cd-113m	Cadmium Group	Eu-155	Trivalents
Cd-115m	Cadmium Group	Eu-156	Trivalents
Sn-117m	Tin Group	Eu-157	Trivalents
Sn-119m	Tin Group	Ra-224	Noble Gas
Sn-121m	Tin Group	Th-228	Tetravalents
Sn-123	Tin Group	U-232	Uranium Group
Sb-125	Cadmium Group	Pa-233	Tetravalents
Sb-126	Cadmium Group		

Chloride Salt Fast Spectrum-1

Nuclide	Corresponding Chemical Group	Nuclide	Corresponding Chemical Group
H-3	New Proposed Group	Te-125m	Chalcogens
As-77	Cadmium Group	Te-133m	Chalcogens
Se-81	Chalcogens	Te-134	Chalcogens
Se-81m	Chalcogens	Xe-131m	Noble Gas
Se-83	Chalcogens	Xe-133m	Noble Gas
Br-83	Halogen	Pr-146	Trivalents
Br-84	Halogen	Pm-147	Trivalents
Kr-83m	Noble Gas	Pm-148m	Trivalents
Nb-93m	Trivalents	Pm-149	Trivalents
Pd-109	Platinoids	Pm-151	Trivalents
Pd-112	Platinoids	Sm-151	Trivalents
Ag-111	Tin Group	Sm-153	Trivalents

Chloride Salt Fast Spectrum-2

Nuclide	Corresponding Chemical Group	Nuclide	Corresponding Chemical Group
Cd-113m	Cadmium Group	Eu-154	Trivalents
Cd-115m	Cadmium Group	Eu-155	Trivalents
Sn-117m	Tin Group	Eu-156	Trivalents
Sn-119m	Tin Group	Eu-157	Trivalents
Sn-121m	Tin Group	U-237	Uranium Group
Sn-123	Tin Group	Pa-233	Tetravalents
Sb-125	Cadmium Group	Pu-242	Tetravalents
Sb-126	Cadmium Group	Cm-243	Trivalents
Sb-128	Cadmium Group	Cm-245	Trivalents
		Cm-246	Trivalents
		Am-242m	Trivalents
		Am-243	Trivalents

Fluoride-Salt-Cooled High Temp Reactors

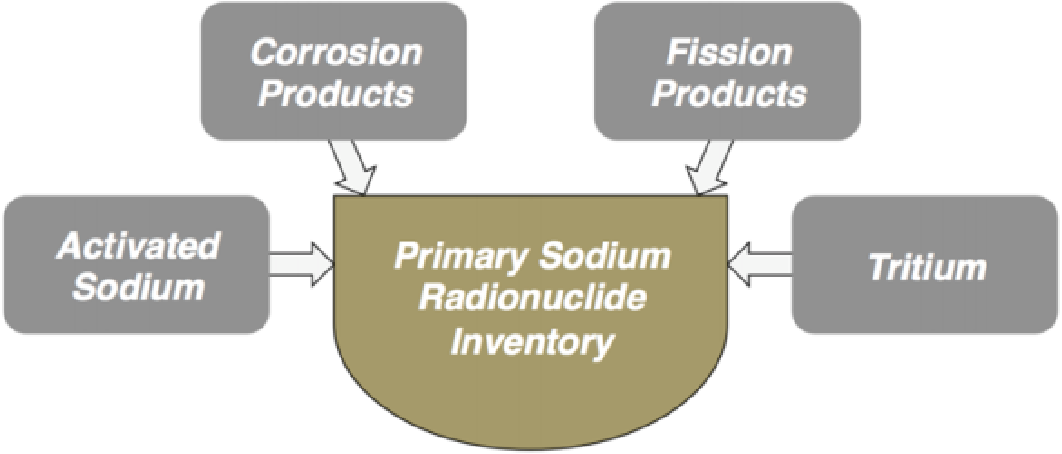
- TRi-structural ISOtropic (TRISO) fuel
- Fluoride-based coolant such as FLiBe
- Low-pressure, high-temperature primary system to deliver heat in the temperature range of 600 – 700 C
- Neutron activation products and fission products generated from defective fuel particles
- Non-noble-gas fission products will have high solubility in the primary coolant, if the fission products form stable fluorides
- Noble metals with low solubility will deposit on the intermediate heat exchanger

FHR Radionuclides of Interest

Element	Isotope	Corresponding Chemical Group
H	3	Proposed New Group
C	14	Proposed New Group
Ag	110m	Tin Group
Sb	125	Cadmium Group
Pm	147	Trivalents
Sm	151	Trivalents
Eu	154	Trivalents
	155	
Pu	242	Tetravalents

Liquid Metal Fast Reactors

- Liquid sodium or lead coolant
- Fast spectrum
- Near-atmospheric pressure
- Analysis utilized information from the Prototype Gen-IV Sodium-cooled Fast Reactor (PGSFR) and the Experimental Breeder Reactor (EBR-II)



The potential source of radionuclides in the Na coolant[19]

LMR Radionuclides of Interest -1

Nuclide	Corresponding Chemical Group	Nuclide	Corresponding Chemical Group
H-3	New Proposed Group	Te-125m	Chalcogens
Na-22	Alkali Metal	Te-133m	Chalcogens
Na-24	Alkali Metal	Te-134	Chalcogens
Ar-41	Noble Gas	Xe-131m	Noble Gas
Cr-51	Early Transition Elements	Xe-133m	Noble Gas
Mn-54	Early Transition Elements	Pr-146	Trivalents
Fe-59	Early Transition Elements	Pm-147	Trivalents
As-77	Cadmium Group	Pm-148m	Trivalents
Se-81	Chalcogens	Pm-149	Trivalents
Se-81m	Chalcogens	Pm-151	Trivalents
Se-83	Chalcogens	Sm-151	Trivalents
Br-83	Halogen	Sm-153	Trivalents
Br-84	Halogen	Eu-154	Trivalents
Kr-83m	Noble Gas	Eu-155	Trivalents
Nb-93m	Trivalents	Eu-156	Trivalents

LMR Radionuclides of Interest - 2

Nuclide	Corresponding Chemical Group	Nuclide	Corresponding Chemical Group
Pd-109	Platinoids	Eu-157	Trivalents
Pd-112	Platinoids	Ta-182	Early Transition Elements
Ag-111	Tin Group	U-237	Uranium Group
Cd-113m	Cadmium Group	Pa-233	Tetravalents
Cd-115m	Cadmium Group	Pu-242	Tetravalents
Sn-117m	Tin Group	Cm-243	Trivalents
Sn-119m	Tin Group	Cm-245	Trivalents
Sn-121m	Tin Group	Cm-246	Trivalents
Sn-123	Tin Group	Am-242m	Trivalents
Sb-125	Cadmium Group	Am-243	Trivalents
Sb-126	Cadmium Group		
Sb-128	Cadmium Group		

Follow-on Activities

- Publication of the initial report on 21 September 2021
- Chemical forms are also included in the report, but for brevity were not included in this presentation
- All radionuclides identified are currently available in MACCS
- Some radionuclides (H-3 and C-14) may require new chemical groups
- Some gaps remain in inventory and experimentation data
- Need to assess the ability for the identified nuclides to migrate into and through the environment
- Need to assess relative importance for offsite consequence analysis
- Need to assess dose coefficients for assessing health consequences

Summary

- MACCS is actively investigating and improving to meet advanced reactor needs!
- Current activities include:
  - Modeling near field dispersion
  - Radionuclide screening
  - MelMACCS update
- A summary was provided of the preliminary radionuclide screening effort
- Follow-on activities underway

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List of Acronyms

EBR	Experimental Breeder Reactor
FHR	Fluoride cooled high temperature reactor
HGTR	High Temperature Gas Reactor
LMR	Liquid Metal Reactor
LWR	Light Water Reactor
MSR	Molten Salt Reactor
PGSFR	Prototype Gen-IV Sodium-cooled Fast Reactor
SOARCA	State-of-the-Art Reactor Consequence Analyses

MACCS 4.0 Revolutionary Improvements

- Optional capability to perform high-fidelity atmospheric transport modeling with HYSPLIT
  - User is responsible for downloading HYSPLIT (from NOAA) and supporting tools (special request to Sandia)
  - Preprocessor steps needed prior to running WinMACCS and MACCS
  - Significantly more computing requirements than the Gaussian model
- Optional state-of-practice, GDP-based model (RDEIM) to account for economic losses (database currently supports contiguous USA)
  - Initially developed prior to 2015
  - Peer review conducted in 2015 led to significant improvements
  - Model was improved and benchmarked between 2015 and 2020
  - Benchmark report published in May 2020
  - Latest version of SecPop supports site data requirements
- Support for special files needed by animation tool, AniMACCS

MACCS 4.0 Evolutionary Improvements

- Limits extended on a large set of input parameters
  - Number of output requests for all output types (999)
  - Number of plume segments using multi-source model (9999)
  - Duration of food ingestion with COMIDA2 (50 yr)
- Convenience enhancements added for cyclical file management
  - Network access
  - Reordering capabilities
  - Creates templates on all valid files
  - Allows source term set per realization when running multi-source model
- Simplified method to eliminate quadratic parameters for the linear-quadratic dose-response model
- Qualifiers can be tab-separated in reports to facilitate importing into a spreadsheet
- Input parameters can be exported, including distribution definitions
- Results for each weather trial are used to define quantile results
- Unused correlations are supported

MACCS 4.1 – Released on 30 July 2021!

- Near-field modeling improvements:
  - SAND2020-2609 compared MACCS v3.11.6 to several near-field atmospheric transport and dispersion codes including QUIC, ARCON96, and AERMOD2
  - Concluded MACCS provides a conservatively bounding assessment in the near-field
  - MACCS v4.1 enhancements added for plume meander and trapping and downwash to simulate or bound near-field assessments of other codes
- New projective peak dose output option
- Documentation added to help menu in WinMACCS
- Updates to the RDEIM economic model
- Mixing layer information for each time period
- Time synchronization
- Pop-up window for converting previous version

Phenomena Treated by MACCS

- Representation of source term
- Atmospheric transport and dispersion
  - Statistical sampling of archived weather data
- Wet and dry deposition
- Exposure pathways to humans
  - Inhalation
  - Cloudshine
  - Groundshine
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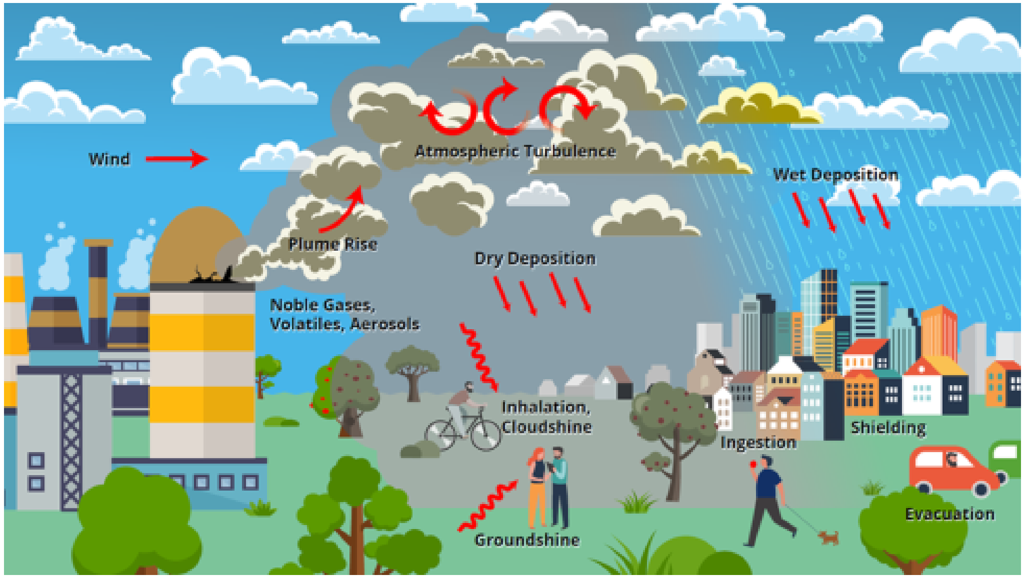

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