| | General Characteristics | | | |
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| 1 | Abstract of Model Capabilities | PC-AQPAC is a Personal Computer-based Air Quality Package which has been designed for use in emergency responses to accidental releases of hazardous substances into the atmosphere. The system predicts hazard zones for potential evacuation. | | |
| | | LFL — Lower Flammability Limit. This defines the minimum concentration of material in air which will support combustion on contact with a source of ignition. The risk of fire is high. In the context of emergency response, this defines a first-priority hazard zone for potential evaluation. | | |
| | | IDLH — Immediately Dangerous to Life or Health. This is defined as the maximum concentration level from which one could escape within 30 minutes without any impairing symptoms or any irreversible health effects. In the context of emergency response this also defines a first-priority hazard zone. | | |
| | | STEL — Short Term Exposure Limit. This is defined as the concentration level to which humans can be exposed continuously for a period of up to 15 minutes without suffering from irritation, chronic or irreversible tissue change, or narcosis of sufficient degree to increase the likelihood of accidental injury, to impair self rescue, or to materially reduce work efficiency, provided that the daily TLV (Threshold Limit Value) is not exceeded. In the context of emergency response this defines a second-priority hazard zone. | | |
| | | TLV — Threshold Limit Value. This is defined as the time-weighted average concentration for a normal 8-hour workday and 40-hour workweek, to which nearly all humans may be repeatedly exposed, day after day, without adverse effect. In the context of emergency response, this defines a third-priority hazard zone. | | |
| | | NOTE: Expert users can change the concentration limits defined in the chemical database. It should also be recognized that PC-AQPAC employs short-range models (<50 km). It should be assumed that a 1 km radius around an accident site represents a first-priority hazard zone for potential evacuation. | | |
| | | Both Gaussian puff and plume models are available for short- and long-term releases, respectively. A heavy gas model is included. The model is designed for rapid field use in an emergency, runs on commonly configured PC hardware and has a large chemical database with toxic limits. | | |
| 2 | Sponsor and/or Developing Organization | AQPAC is a chemical and radiological consequences code originally written by the Atmospheric Environment Service (AES) of the Canadian Government. | | |
| 3 | Last Custodian/ Point of Contact | Dr. Dan McGillvray 64 Ferris Road Toronto, Ontario, Canada M4B164 (416) 285-9305 | | |
| | | Dr. Sam M. Daggupaty Atmospheric Environmental Service 4905 Dufferin Street Downsview, Ontario, Canada M3H 5T4 (416) 739-4451 sam.daggupaty@tor.ec.gc.ca primary individual | | |
| 4 | Life-Cycle | It has been modified over the past several years and is now offered commercially with an enhanced user interface. | | |

| 5 | Model Description Summary | PC-AQPAC provides menu-driven access to the following models, databases and modules. Source strength model which computes the rate and type of emission (instantaneous or continuous) and automatically selects the appropriate dispersion model (or models) to run. Expert users have the option to override the selections made by the source strength model. Heavy gas puff and plume models which predict the dispersion and concentration of heavier-thanair gases. Output data are presented in both graphical and tabular form. Neutral gas puff and plume models which predict the dispersion, depletion and ground deposition, as well as the atmospheric concentration of lighter-than-air gases as well as radioactive gas clouds, forest fire smoke particles, airborne viruses, etc. Output data are presented in both graphical and tabular form. Chemical database which contains detailed information on over 75 hazardous substances (including radioactive materials) and facilitates the entry of new chemical data into the database. Meteorological database which contains more than five worst-case and common case weather conditions and may be easily added to or updated with "nowcast." |
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| 5 | Model Description Summary (Cont.) | Emergency response report module which guides the user through a series of questions concerning an accident and maintains an official record for review after the accident. Review module for reviewing both graphical and tabular output from the PC-AQPAC models. The review module also provides access to the graphical interface which allows the user to print (or reprint at different scales) selected graphical output. |
| 6 | Application Limitation | Straight-line plume, invariant meteorology and source term, no topographical effects, no fires or chemical reactions. The model does include plume depletion and deposition. There is no mention of building wake or downwash models for close-in calculations. Several simplifying assumptions are made in the source term model such as constant pool diameter for liquid spills. |
| 7 | Strengths/ Limitations | Straight-line plume, invariant meteorology and source term, no topographical effects, no fires or chemical reactions. The model does include plume depletion and deposition. There is no mention of building wake or downwash models for close-in calculations. Several simplifying assumptions are made in the source term model such as constant pool diameter for liquid spills. |
| 8 | Model References | Colenbrander, G.W., 1980: A mathematical model for the transient behavior of dense vapour clouds, Third International Symposium on Loss Prevention and Safety Promotion in the Process Industries, Basle, Switzerland, September 15–19, 1980. Colenbrander, G.W. and J.S. Puttock, 1983: Dense gas dispersion behavior: Experimental observations and model development, 4th International Symposium on Loss Prevention and Safety Promotion in the Process Industries, Harrogate, England, September 12–16, 1983. Daggupaty, S.M., 1990: A source strength model for accidental release of hazardous substances, Proceedings of the 7th Annual Technical Seminar on Chemical Spills, June 4–5, 1990, published by the Minister of Supply and Services, 55–60. Havens, J.A. and Spicer T.O., 1985: Development of an atmospheric dispersion model for heavier-than-air mixtures, University of Arkansas, Department of Chemical Engineering, Final Report under Contract No. DT-CG-23-80-C-20029, prepared for the U.S. Coast Guard, Washington, D.C. Matthias, C.S., 1990: Dispersion of a dense cylindrical cloud in calm air, Journal of Hazardous Materials, 24: 39–66. Matthias, C.S., 1992: Dispersion of a dense cylindrical cloud in a turbulent atmosphere, Journal of Hazardous Materials, 30: 117–150. Turner, D.B., 1964: A diffusion model for an urban area, Journal of Applied Meteorology, 3: 83–91. |
| 9 | Input Data/Parameter Requirements | Input of weather data can be manual or automatic using an appropriate digital interface with a source of meteorological data. A minimum of information is required for a run since data for a relatively large number (75) of common toxic chemicals is built in. |
| 10 | Output Summary | Output is both printed and graphical, showing the downwind and lateral area where toxic limits are exceeded. Each run is separate with its own meteorological and source data. No indication of error or diagnostic messages was found in the user's manual. Setup time is minimal. |
| 11 | Applications | Primarily developed as an emergency response model. May have been used for other applications. |
| 12 | User-Friendliness | Appears to be easy to run based on review of demo only. |
| 13 | Hardware-Software Interface Constraints/ Requirements | Computer operating system: DOS 4.0 or higher on PC. Computer platform: Disk space requirements: 5 MB Run execution time (for a typical problem): No runs were made. Programming language: Believed to be FORTRAN (original version.) Other computer peripheral information: Appears to be easily installed on PC. |

| 14 | Operational Parameters | Identify whether the code has any error diagnostic messages to assist the user in troubleshooting operational problems: No error diagnostics. | | | |
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| 15 | Surety Considerations | Benchmark test and comparison with field experiments have been made with good results. | | | |
| | | Specific Characteristics | | | |
| Part A | A: Source Term Submod | del Type | | | |
| A1 | Source Term Algorithm? | _✓YESNO | | | |
| A2 | For Chemical Consequence Assessment Models | Liquid spill: pool evaporation particulate resuspension Pressurized releases: two-phase jets _v _ flashing entrainment aerosol formation Solid spills: _v _ resuspension sublimation. | | | |
| Part I | B: Dispersion Submode | I Туре | | | |
| B1 | Gaussian | <u>✓</u> Straight-line plumeSegmented plume Statistical plume Statistical puff | | | |
| B2 | Similarity | Plume Puff | | | |
| Part (| C: Transport Submodel | Туре | | | |
| C2 | Deterministic | Yes | | | |
| C4 | Frame of Reference | <u>✓</u> Eulerian Lagrangian Hybrid Eulerian-Lagrangian | | | |
| Part I | D: Fire Submodel Type (| (Not Applicable) | | | |
| Part I | E: Energetic Events Sub | emodel Type (Not Applicable) | | | |
| Part I | : Health Consequence | Submodel Type | | | |
| F1 | For Chemical Consequence Assessment Models | Health effects:fatalitiescancerslatent cancerssymptom onset Health criteria IDLHSTELTLVTWAERPGTEELAEGLWHO Zones with flammable limits:UFLLFL Blast overpressure regions: Fire radiant energy zones: Risk qualification: Concentration: single value time-history integrated dose Probits: | | | |
| Part G: Effects and Countermeasures Submodel Type (No Information Provided.) | | | | | |
| | H: Physical Features of | | | | |
| H2 | Release Elevation | <u>✓</u> ground <u>✓</u> roof | | | |
| H6 | Mixing Layer | trapping lofting✓ reflection penetration inversion breakup fumigation temporal variability | | | |
| H7 | Cloud Buoyancy | <u>✓</u> neutral [passive] <u>✓</u> dense [negative] <u>✓</u> plume rise [positive] | | | |
| H10 | Deposition | gravitational settingv dry deposition precipitation scavenging resistance theory deposition simple deposition velocity liquid deposition plateout and re-evaporation | | | |
| Part I: Model Input Requirements | | | | | |
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| 11 | Radio(chemical) and Weapon Release Parameters | Release rate: Continuous Time dependent Instantaneous Release container characteristics: vapor temperature tank diameter tank height tank temperature tank pressure pipe length Jet release: initial size shape concentration profile at end of jet affected zone Release dimensions: point line area Release elevation: ground roof stack | | |
|--------|---|--|--|--|
| 12 | Meteorological Parameters | Wind speed and wind direction:v_single point single tower/multiple point multiple towers Temperature: _v_ single point single tower/multiple point multiple towers See above. Dew point temperature: single point single tower/multiple point multiple towers Precipitation: single point single tower/multiple point multiple towers See above. Turbulence typing parameters: temperature difference sigma theta sigma phi Monin-Obukhov length roughness length v_ cloud cover v_ incoming solar radiation user-specified Four dimensional meteorological fields from prognostic model: | | |
| Part J | Model Output Capab | ilities | | |
| J1 | Hazard Zone | Area above LEL is plotted on screen. | | |
| J2 | Graphic Contours and Resolution | Plots for different limits. | | |
| J3 | Concentration Versus Time Plots | Concentration isopleths only. | | |
| J4 | Tabular at Fixed Downwind Locations | Yes | | |
| J5 | Health Effects | <u>✓</u> toxicity indices [e.g., ERPG's, PAG's] potential fatalities cancers other adverse effects | | |
| Part K | Part K: Model Usage Considerations (No Information Provided.) | | | |